

(19) World Intellectual Property  
Organization  
International Bureau



(43) International Publication Date  
29 April 2004 (29.04.2004)

PCT

(10) International Publication Number  
**WO 2004/035812 A2**

(51) International Patent Classification<sup>7</sup>: **C12Q 1/00**

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(21) International Application Number:  
PCT/GB2003/004492

(22) International Filing Date: 16 October 2003 (16.10.2003)

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(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:  
0224102.4 16 October 2002 (16.10.2002) GB  
0226598.1 14 November 2002 (14.11.2002) GB

(81) Designated States (*national*): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

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(84) Designated States (*regional*): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

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Published:

— *without international search report and to be republished upon receipt of that report*

*For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.*

WO 2004/035812 A2

(54) Title: HYDROXYLASES AND MODULATORS THEREOF

(57) Abstract: A method of identifying, screening, characterising or designing a chemical entity, which mimics or binds to FIH, is described. The method comprises comparing a structural model of FIH with a structural model for said chemical entity, wherein said structural model of FIH is derived from structural factors or structural coordinates determined by subjecting to X-ray diffraction measurements a crystal comprising FIH. Such chemical entities may be used in the treatment of a condition associated with increased or decreased HIF levels or activity.

## HYDROXYLASES AND MODULATORS THEREOF

### Field of Invention

The present invention relates to methods of designing inhibitors of FIH using  
5 the crystal structure of FIH, and to inhibitors of FIH and their use in the treatment of  
ischaemia.

### Background of the Invention

In cells of many organisms exposure to an environment in which oxygen is  
10 depleted relative to optimal levels induces a hypoxic response. In these hypoxic  
cells, activation of a transcriptional cascade involving hypoxia inducible factor (HIF)  
directs a series of adaptive responses that enhance oxygen delivery or limit oxygen  
demand. Activation of HIF in cancer and ischaemic hypoxic vascular diseases has  
revealed its important role in human pathology and demonstrated that manipulation  
15 of HIF activity has important therapeutic potential.

The HIF transcriptional complex comprises an  $\alpha\beta$  heterodimer, HIF- $\beta$  being a  
constitutive nuclear protein that dimerises with oxygen regulated HIF- $\alpha$  subunits  
(Semenza, G. L. (2000) *Genes Dev.* **14**, 19831991). The activity of HIF- $\alpha$ , is  
suppressed by oxygen-dependent modification catalysed by a series of Fe<sup>(II)</sup> and 2OG  
20 dependent dioxygenases that hydroxylate specific HIF- $\alpha$  residues. In the presence of  
oxygen in human HIF-1 $\alpha$ , 4-hydroxylation of Pro402 or Pro564 by a set of HIF  
prolyl hydroxylase isozymes (PHD1-3) (Epstein et al. (2001) *Cell* **107**, 4354; Bruick,  
R. K., and McKnight, S. L. (2001) *Science* **294**, 13371340) mediates its recognition  
by the von Hippel-Lindau (VHL) ubiquitin ligase complex and consequent targeting  
25 for proteasomal destruction (Ivan et al, (2001) *Science* **292**, 464468; Jaakkola et al  
(2001) *Science* **292**, 468472, WO 02/074981). In a complementary mechanism FIH  
catalyses  $\beta$ -hydroxylation of HIF-1 $\alpha$  Asn803 (Lando et al, (2002) *Science* **295**,  
858861) blocking interaction with the transcriptional co-activator p300 (Dames et al.,  
(2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 52715276; Freedman et al, (2002) *Proc.*  
30 *Natl. Acad. Sci. U. S. A.* **99**, 53675372). In hypoxia, limitation of enzymatic activity  
allows HIF- $\alpha$  to escape destruction and become transcriptionally active.



Inhibition of HIF hydroxylases strongly activates the HIF transcriptional cascade even in the presence of oxygen (Epstein et al.(2001) *Cell* **107**, 4354). Thus, inhibition of the HIF hydroxylases results in a pro-angiogenic response that may be used in the treatment of cardiovascular diseases/ ischaemic hypoxic vascular diseases including myocardial infarction and anaemia. A problem with this approach is that the human cells contain other enzymes belonging to the same family as the HIF hydroxylases, i.e. utilising dioxygen (a cosubstrate), 2-oxoglutarate (2OG) (a cosubstrate) and Fe(II) (a cofactor). Such enzymes are exemplified by phytanoyl coenzyme A hydroxylase, procollagen prolyl-4-hydroxylase, procollagen prolyl-3-hydroxylase, gamma-butyrobetaine hydroxylase, Alk B (a DNA repair enzyme) and others including predicted 2OG oxygenases identified on the basis of sequence analyses including a sub-family related to FIH (Hewitson et al., *J BIOL CHEM* **277** (29): 26351-26355, 2002). It is generally agreed that it is desirable that enzyme inhibitors used as pharmaceuticals are selective for their intended target or the targets involved in producing the desired effect. A lack of selectivity can lead to toxic side effects that render particular compounds unsuitable for use in human or animal therapy. One approach to identifying compounds that are selective for the intended target is to undertake structural, mechanistic and other analyses on the intended agents and to use the information gained to aid in the preparation of selective compounds, or more selective compounds (relative to those previously known), for use as pharmaceuticals for use in humans or animals. Here we describe structural and other studies on the HIF hydroxylases that enable the design of selective inhibitors of FIH and related enzymes.

## Summary of the Invention

The present inventors have now identified the site of hydroxylation of asparagine 803 of HIF-1 $\alpha$  by FIH. In addition, the inventors have obtained the crystal structure for FIH including identification of the binding site and residues involved in the interaction of FIH with HIF.

Accordingly, the present invention provides a method of identifying, screening, characterising or designing a chemical entity which mimics or binds to FIH, which method comprises comparing a structural model of FIH with a structural

model for said chemical entity, wherein said structural model of FIH is derived from structural factors or structural coordinates determined by subjecting to X-ray diffraction measurements a crystal comprising FIH.

The invention also provides for:

- 5           -       the use of the structural co-ordinates obtainable by subjecting a crystal comprising FIH to X-ray diffraction measurements and deducing the structural co-ordinates from the diffraction measurements, to identify, screen, characterise, design or modify a chemical entity;
- a chemical entity identified by a method of the invention, wherein
- 10       said chemical entity inhibits the asparaginyl hydroxylase activity of FIH; and
- a chemical entity of the invention for use in a method of treatment.

#### Description of the Figures

Figure 1: 2OG binding site.

15   Figure 2: binding of Asn-803.

Figure 3: conformation of CAD at site 1.

Figure 4: conformation of CAD at site 2.

Figure 5: figure indicating the turn formed by 802-804 of HIF-CAD at the active site of FIH.

20   Figure 6: conformation of the turn formed by residues 802-804 of HIF-CAD at the active site of FIH.

#### Detailed Description of the Invention

The present inventors have identified the position of asparagine 803 that is

25   hydroxylated by FIH. In addition, the inventors have identified the crystal structure of FIH. This structure therefore allows for identification of the amino acid residues involved in binding of FIH to HIF.

The identification of the interaction and the structures allows for the characterisation or identification of chemical entities which can bind and in particular

30   which can inhibit FIH. A number of different types of inhibitors can be identified as discussed in more detail below.

The inventors have successfully crystallised human FIH. This the first crystallisation of FIH and has enabled determination of the crystal structure. Co-ordinates from the crystal analysis are set out in Table 3 below. The studies have allowed analysis of the binding of asparagine-803 of HIF and analysis of the conformation of the c-terminal activation domain (CAD) of HIF at the binding sites to FIH. The present invention provides the use of the structural co-ordinates of FIH to identify, characterise, design or screen chemical entities. The chemical entities of interest are those which bind to FIH and in particular which inhibit the asparaginyl hydroxylase activity of FIH. In addition, chemical entities may be identified, characterised or designed which are modified asparagine hydroxylases.

Typically, the structural co-ordinates used are obtainable by subjecting a crystal comprising FIH or a fragment thereof to X-ray diffraction measurements and deducing the structural co-ordinates from the diffraction measurements, to identify, screen, characterise, design or modify a chemical entity. The structural co-ordinates indicate the positions of individual atoms within the crystal and give an indication of the space available for adjusting the position of individual atoms when designing a chemical entity.

The crystal subjected to X-ray diffraction methods comprises FIH or a fragment thereof. The FIH may be from any source but is preferably human FIH. The FIH may be a modified form. For example, the FIH may be modified by insertion, deletion, n-terminal or C-terminal addition, or substitution of amino acid by another amino acid. Amino acid substitutions may be conservative substitutions. Typically, when crystallised, a FIH mutant will adopt a similar 3-dimensional structure to that adopted by the corresponding FIH. A mutant may be an inactive FIH.

References to FIH herein refer to FIH and homologues thereof. Amino acid residues are defined with reference to the position in FIH (see e.g. Hewitson et al). The relevant amino acid residues of homologues of FIH are the equivalent amino acid residues, based on for example the best alignment of homologue to FIH.

A FIH may be isolated by any suitable means for use in crystallisation studies. For example, a FIH may be purified using biochemical means from a suitable source. Typically, however, it will be convenient to over express FIH in cells and purify FIH from those cells. Thus, a polynucleotide encoding a FIH may be used

in the construction of a vector. The FIH may be crystallised according to any method known to those skilled in the art. X-ray diffraction may be carried according to any suitable method. The data collected from X-ray diffraction experiments may be processed to deduce the structural co-ordinates of FIH using any suitable method.

5       The invention provides the use of structural co-ordinates to identify, characterise, design or screen a chemical entity. The chemical entity may be one which binds to FIH, or which acts as an inhibitor of asparaginyl hydroxylase activity. Alternatively, the chemical entity may be a modified FIH to alter the activity of a FIH.

10       A chemical entity which binds to or inhibits FIH is any chemical entity capable of forming an association with the FIH. The binding or inhibition may be non-specific, for example, such an entity may also bind to or inhibit other 2OG oxygenases. Alternatively, an agent may be designed or identified which specifically binds to or inhibits asparaginyl hydroxylases. An agent may be designed or identified  
15       which is a specific inhibitor of FIH, but not other asparaginyl hydroxylases.

      The structural co-ordinates of FIH allows a skilled person to predict which amino acids are important in active site formation and which amino acids are important in contacting the substrate. The substrate binding site may be shown as a 2 dimensional representation or a 3 dimensional representation produced by physical  
20       models or displayed on a computer screen. Such representations can be used to design, identify or screen chemical entities which bind to or inhibit or are predicted to bind to or inhibit FIH. Such representations can also be used to identify modifications of FIH to alter its activity characteristics.

      Examples of modifications to FIH include modifications to increase the  
25       binding of FIH for its substrate, or to alter the substrate the specificity. Alternative modifications include those which alter the activity of FIH, for example, to remove asparaginyl hydroxylase activity.

      The representations of the structures may be used in other ways. For example, the representations of the FIH active site may be used to model constraints  
30       by the putative introduction of covalent bonds between the atoms which come close together when FIH binds to a substrate. Representation of the active site may be used to predict which residues of FIH are likely to be involved in steric hindrance.



Such residues may be modified, replaced or deleted to decrease esoteric hindrance in order to increase avidity of the peptide for its substrates.

In general, it will be necessary to process the structural co-ordinates obtainable according to the invention in computer-based methods in order to identify or design chemical entities with the desired molecular structure or to identify chemical entities whose structure is complementary to all or part of another chemical entity of interest. Thus, chemical entities which have a structure similar to FIH may be identified or designed. Chemical entities which bind to FIH may be identified or designed. Preferably, such chemical entities bind at the active site of FIH and in general may act as inhibitors of asparaginyl hydroxylase activity.

Such computer-based methods fall into two broad classes: database methods and *de novo* designed methods. In database methods, the chemical entity of interest is compared to all chemical entities present in a database of chemical structures and chemical identities whose structure is in some way similar to the compound of interest identified. The structures in the database are based either on experimental data, generated by NMR or X-ray crystallography, or models of 3 dimensional structures based on 2 dimensional data. In *de novo* design methods, models of chemical entities, for example such are those which might bind to FIH are generated by a computer program using information derived from known structures and/or theoretical rules.

Similarly, the FIH structural coordinates may be used to screen for the expected activity of chemical entities selected, designed or shown to be modulators such as inhibitors of other hydroxylases, for example prolyl hydroxylases. For example the compounds may be screened to assess the likelihood of a prolyl hydroxylase inhibitor additionally inhibiting FIH hydroxylase. Such screening methods may be useful in identifying agents which selectively inhibit HIF prolyl hydroxylase, but not HIF asparaginyl hydroxylase.

Chemical entities designed or selected according to the methods of the invention may be tested and optimised using computational or experimental evaluation. Experimental methods to assay for the activity of asparaginyl hydroxylase are described in more detail below.

Based on the structure of FIH, a number of different types of inhibitors can be identified. These inhibitors are discussed in more detail below.

#### Dimerisation inhibitors

5       The crystallographic asymmetric unit contains one FIH molecule. However, analysis of crystallographic symmetry revealed a dimeric form of FIH, consistent with native gel-electrophoresis analysis. The dimer interface involves the two C-terminal helices of each molecule in an interlocking arrangement predominantly involving hydrophobic interactions. This unusual interface buries a surface area of  
10   3210 Å<sup>2</sup>, large on average by comparison to other dimeric proteins of this size. Inhibitors of dimerisation include those that bind to residues that form the dimerisation interface including residues selected from 330-346, such as Leu-340 and Ile-344. Inhibitors include peptides or peptide mimetics that correspond to all or part of the FIH residues involved in the dimerisation interface.

15       For example, such inhibitors may comprise a fragment of FIH, for example, including the residues from 340 to 344, preferably, including residues 330 to 346. Such a fragment may typically have 6 or 10 amino acids in length, preferably, up to 15 or 20 amino acids in length. Alternatively, peptide homologues may be used, for example, which comprise a homologue to the residues of 340 to 344 or 330 to 336,  
20   including 1, 2 or more substitutions. Additional agents include peptides or peptide mimetics which can be designed based on the crystal structure to interfere with dimerisation.

#### Inhibitors exploiting metal binding in FIH:

25       The structural work defines the presence of Fe(II) at the active site of FIH and by implication related HIF hydroxylases. The iron is bound in an almost octahedral manner by the side chains of His199, Asp201 and His279, the 2-oxo and 1-carboxylate groups of 2OG. In the enzyme-substrate complexes there is a vacant position opposite His279 revealing that the enzyme is primed for dioxygen binding.  
30   Accommodation of a ligand opposite His279 may require disruption of the hydrogen bond between Asp201 and CAD Asn803 (the iron and Asn803 β-carbon are only ~4.9 Å apart). Subsequent decarboxylation of 2OG presumably yields an iron-oxo

species  $[\text{Fe}^{(\text{IV})}=\text{O} \leftrightarrow \text{Fe}^{(\text{III})}-\text{O}\cdot]$  that effects oxidation at the carbon of Asn-803 in the C-terminal transactivation domain (CAD) of HIF.

Compounds that contain functional groups that bind to iron are useful as inhibitors of FIH. Examples of such compounds include thiols, alcohols, phenols including flavonoids such as quercitin and derivatives thereof, carbohydrates, hydroxamates, imidazoles and other heterocycles for example nitrogen containing heterocycles.

$\text{Zn}^{(\text{II})}$  binds to FIH in an identical manner to  $\text{Fe}^{(\text{II})}$  (structure 3), consistent with the metal-mediated hypoxic effect being due to displacement of  $\text{Fe}^{(\text{II})}$  from the active site of HIF hydroxylases. Since neither  $\text{Zn}^{(\text{II})}$  nor other metal inhibitors of FIH can replace  $\text{Fe}^{(\text{II})}$  as a cofactor in catalysis, compounds that preferentially promote the binding of a metal other than iron [such as  $\text{Zn}^{(\text{II})}$ ] at the active site of FIH act as inhibitors.

A further class of inhibitor are non-metallic inhibitors that operate via competing with  $\text{Fe}^{(\text{II})}$  for binding at the active site. Such inhibitors may bind to any or all of the triad of residues (His-199, Asp-201, His-279), that bind the  $\text{Fe}^{(\text{II})}$  at the active site of catalytically active FIH.

#### Inhibitors exploiting the 2OG binding sites

The FIH:CAD structures with NOG reveal that like 2OG it is ligated to iron in a bidentate manner and imply it is an inhibitor due to decreased susceptibility to attack by an iron bound (su)peroxide intermediate or by hindering binding of dioxygen to the metal.

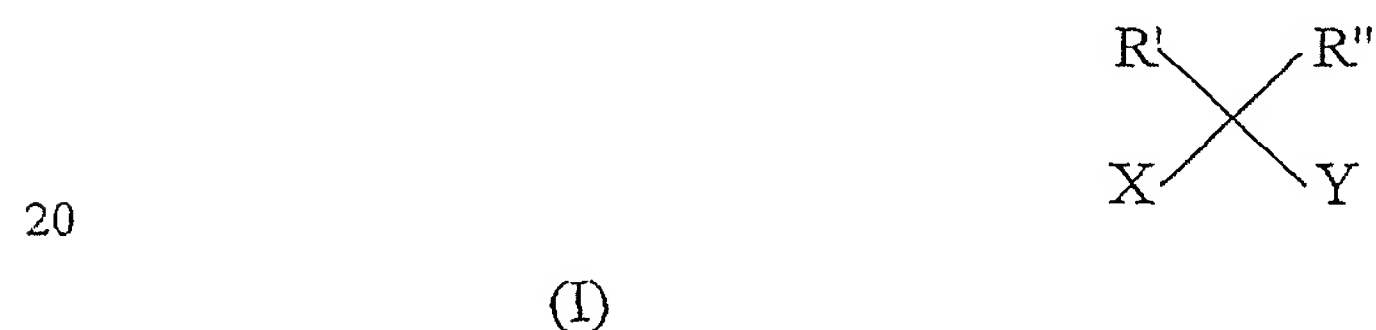
The structural studies on FIH reveal the binding interactions for the 2OG and NOG (see for example Figure 1). The 5-carboxylate of 2OG (and the equivalent carboxylate of NOG) forms hydrogen bonds with the side-chains of Lys214, Thr196 and Tyr145; such interactions are unprecedented in other structures of 2OG oxygenases. FIH is further unusual in that Lys214 is on the fourth DSBH (double stranded beta-helix)  $\beta$ -strand whereas previously assigned basic 2OG-5-carboxylate binding residues are at the beginning of the eighth DSBH strand.

The structural studies reveal the FIH residues that form the pocket into which 2OG and NOG bind. In addition to the aforementioned these include the side-chains

of Ile-281, Leu-186, Leu-188, Phe-207, Thr-196. Knowledge of these interactions enables the design of improved (as measured by binding parameters) and selective inhibitors. Thus, for example an inhibitor binding in the 2OG binding pocket may form hydrophobic interactions with any or all of the side chains of Ile-281, Leu-186  
 5 Leu-188, Phe-207, Thr-196. Further it may form electrostatic or hydrogen bonding interactions with the residues involved in binding the 5-carboxylate of 2OG (Lys214, Thr196 and Tyr145).

Selective inhibition of FIH via inhibitors interacting with the 2OG binding residues is exemplified as follows: kinetic analyses of a series of inhibitors based  
 10 upon *N*-oxaloyl amino acids revealed the *R*-enantiomer ( $IC_{50}$  0.4 mM) of *N*-oxaloylalanine was significantly more potent than the *S*-enantiomer ( $IC_{50}$  2.5 mM). Analysis of the 2OG binding pocket in FIH reveals that the binding of the *S*-enantiomer is hindered by interactions between its methyl group and the side chain of Thr-196 and, Ile-281 in the 2OG binding pocket. A reversed selectivity (i.e. the *S*-  
 15 enantiomer was more potent) was observed both for procollagen prolyl-hydroxylase and the PHD isozymes, demonstrating it should be possible to develop selective inhibitors for individual types of HIF hydroxylase. Such inhibitors may or may not chelate to an active site metal.

Compounds include those of general formula

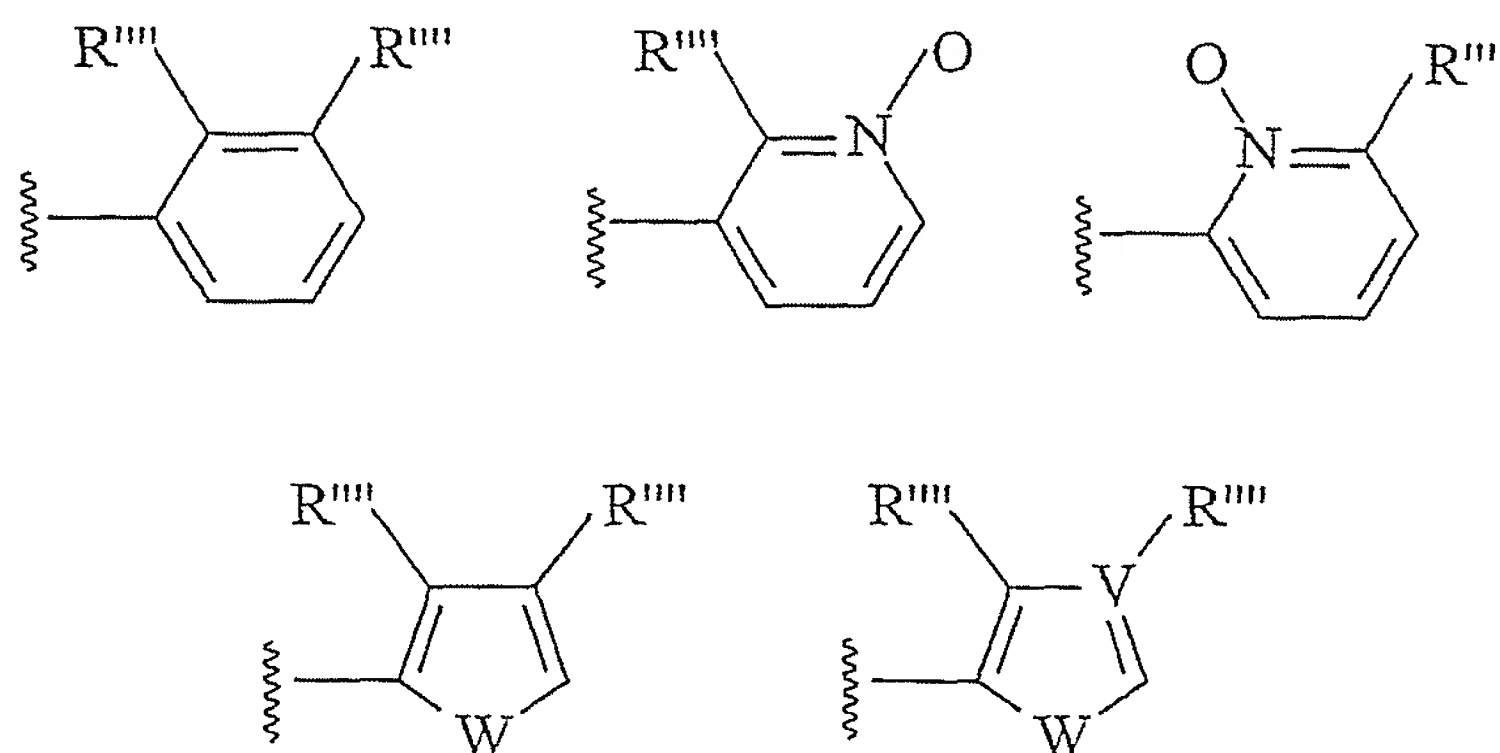


wherein each of  $R'$  and  $R''$ , which may be the same or different, is H, F or  $C_1$  to  $C_3$  alkyl or substituted alkyl,  $CH_2OH$ ,  $CH_2CO_2H$  or  $CONH_2$ , X is  $COOH$ ,  $SOOH$ , or  
 25  $CONHH$  or an ester thereof, or heterocyclic or other group which forms a favourable interaction with one or more of the side chains of Lys-214, Thr-196 and Tyr-145, i.e. those residues involved in binding the 5-carboxylate of 2OG as revealed in the crystallographic analyses,  
 Y is  $-(CR'''R''')_nZ$ , where Z is



- NR'''COCOOH, -NR'''CSCOOH, -NR'''COCOSH,  
 - CHSR'''CONR'''R''', -CHOR'''CONR'''OR''', -CHSR'''CONR'''OR''' or  
 - CHOR'''CONR'''NR'''OR''', wherein each R''', which may be the same or  
 different, is H, alkyl, OH or O-alkyl, n is 0 to 3 and preferably 0, or

5



10 wherein R'''' is OH, OR''' or NHCOR''', and W is S, NH, or O.

Thus X is a group that forms favourable interactions with one or more of the  
 side chains of interactions one or more of the side chains of Lys-214, Thr-196 and  
 Tyr-145, i.e. those residues involved in binding the 5-carboxylate of 2OG. X may be  
 functionalised as a pro-drug such that is delivered to the desired site of action or has  
 15 desirable pharmacokinetic properties. As indicated above, X can be an ester such a  
 methyl or ethyl ester or amide derivative of carboxylic acid versions of X.

If n is 0, Y is typically CONHOH, CONHNH<sub>2</sub>, NR'''COCOOH,  
 NR'''CSCOOH or NR'''COCOSH. Y is preferentially of a size such that it can  
 chelate to the active site metal whilst maintaining all or some of the favourable  
 20 binding interactions found in the 2OG binding pocket as defined by crystallographic  
 analyses. As with X, Y may be functionalised as a pro-drug.

When Y contains an aromatic ring as indicated above it can comprise other  
 ring systems including aryl or functionalised aryl rings as well as heterocyclic and  
 functionalised heterocyclic rings. The above rings may be further functionalised to  
 25 optimise binding at the FIH active site.

Inhibitors exploiting the peptide substrate binding siteThere are two binding sites

The ES complex structures unexpectedly reveal two separate binding sites involving CAD<sub>795-806</sub> (i.e residues 795-806 of the C-terminal transactivation domain of HIF) (Site 1) and CAD<sub>813-822</sub> of HIF (Site 2) with contact surface areas of 1640 Å<sup>2</sup> and 1080 Å<sup>2</sup>, respectively (see for example the figures). CAD residues in these regions are conserved in all known HIF-1α and HIF-2α sequences. The electron density for site 1 was of good quality, with only the side-chain of Tyr798 poorly defined, while that for site 2 was at a lower level and quality, probably reflecting weaker binding at this site. CAD<sub>804-806</sub> and presumably also CAD<sub>807-811</sub>, for which density was not observed, do not form direct interactions with FIH. Kinetic analyses employed to investigate the relative importance of Sites 1 and 2, revealed that fragments containing site 1 only are hydroxylated by FIH but less efficiently than those containing both sites demonstrating that both are important in binding and that both may be exploited in inhibition studies.

At Site 1 CAD<sub>795-803</sub> are bound in a groove and adopt a largely extended conformation linked to FIH by ten hydrogen bonds. Asn803 of CAD is strikingly buried at the active and directly adjacent to the Fe<sup>(II)</sup>. CAD Asn803 and Ala804 form a tight turn, stabilised by a hydrogen bond between the backbone carbonyl of Val802 and NH of Ala804, which projects the side chain of Asn803 towards the Fe<sup>(II)</sup>. The side chain of CAD Asn803 is precisely orientated by three hydrogen bonds to enable hydroxylation at the *pro-S* position of the β-carbon consistent with the NMR assignments (see above) The primary amide of CAD Asn803 is sandwiched between FIH residue Tyr102 and the Fe<sup>(II)</sup>, and forms hydrogen bonds with the side chains of FIH residues Gln239 and Arg238, residues located on the insert to the DSBH motif. Significantly, the substrate and Fe<sup>(II)</sup> binding sites are directly linked since the backbone nitrogen of CAD Asn803 also forms a hydrogen bond (~3 Å) with the carboxylate oxygen of Asp201 that is not complexed to the iron. Six additional hydrogen bonds stabilise the binding of FIH to CAD<sub>795-801</sub>.

In contrast with Site 1, Site 2 is located on the FIH surface and involves only two hydrogen bonds. CAD<sub>816-823</sub> of Site 2 form an α-helix, in exact agreement with the structure of this region in complex with CBP/p300 (Dames et al., (2002) *Proc.*

*Natl. Acad. Sci. U. S. A.* **99**, 52715276; Freedman et al, (2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 53675372). As in that complex, the highly conserved Leu818, Leu819 and Leu822 sit in a hydrophobic pocket on the surface of FIH and form the basis of the binding interaction and so it is not possible for these residues to bind  
5 simultaneously to CBP/p300 and FIH.

The extended loop conformation adopted by the CAD residues at Site 1, contrasts with the  $\alpha$ -helical conformation adopted by the same residues when complexed with the 1st transcriptional adaptor zinc-binding domain (TAZ1) of CBP/p300(Dames et al.,(2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 52715276;  
10 Freedman et al, (2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 53675372). The disordered structure observed for the CAD, and other HIF- $\alpha$  residues, when free in solution may thus reflect a requirement to adopt more than one conformation for complex formation with different proteins.

The changes in the conformation of CAD on binding are complemented by  
15 changes in FIH revealing an induced fit binding process; Trp296 of FIH undergoes a 50° rotation about C<sub>beta</sub>-C<sub>alpha</sub> to accommodate CAD Val802, while both Tyr102 and Tyr103 become more ordered. Further evidence of induced fit comes from the significant differences in resolution between the structures obtained with and without CAD fragments bound reflecting ordering of FIH that occurs on binding (structure 4,  
20 for comparison, represents FIH complexed with Fe<sup>(II)</sup> and 2OG alone). Interference in the conformational changes involved in the hypoxic response, in particular those involving the CAD region, e.g. by use of small molecules or by gene or protein therapy, may allow manipulation of the hypoxic response to enable pro or anti-angiogenetic responses.

25 Thus, the structural studies define the (i) FIH residues involved in binding the CAD of HIF (ii) conformation of FIH when CAD is bound and (iii) conformation of CAD when bound to FIH. These results are useful in the design of selective inhibitors of FIH and related enzymes. Features of the FIH binding sites may be used to mediate tighter binding of inhibitors to FIH or to obtain inhibitors that do not bind  
30 tightly to FIH, i.e. avoid inhibition of FIH.

Inhibitors binding at or close to the Site 1 may exploit electrostatic, hydrogen binding and/or hydrophobic interactions with Tyr-102, Asp-104, Lys-106, Asp-201,

Glu-202, Gln-147, Gln-239, residues 299-303, His-313, Ala-317, Ile-318, Asn-321, Lys-324, Arg-238, Trp-296, Asn-321- Lys-324. Inhibitors binding at Site 1 may mimic or partially mimic the turn conformation adopted by CAD when bound at Site 1.

5        Inhibitors binding at or close to Site 2 may exploit electrostatic, hydrogen binding and/or hydrophobic interactions with residues Thr-149, Leu-150, Asn- 151, Asp-152 and residues Val-159, Phe-162, Leu-163, Trp-167, Gln-181, Leu-182, Thr-183, Ser- 184, Asn- 185. Inhibitors binding at Site 2 may mimic or partially mimic the helical conformation adopted by CAD when bound at Site 2.

10        It is recognised that inhibitors need not bind to both Sites 1 and 2, although that they may, and that Site 1 is preferred over Site 2.

Residues 801 – 805 of CAD that bind at Site 1, and in particular residues 802-805 form a turn conformation in which the distance of the backbone C=O of 802 to the backbone NH of 804 is ca. 2.8 Å. Including the H-bond formed between the NH  
15        of Ala-804 and the carbonyl O of Val-802 of the HIF-1alpha CAD, the turn contains 7 atoms in a pseudo-ring.

Turns are especially amenable to mimicry by analogues useful for enzyme inhibition or receptor binding. The medicinal chemistry literature is replete with examples of such turn mimics. These can be modified by known methods to bind to  
20        specific targets, in particular given the knowledge of the target structure.

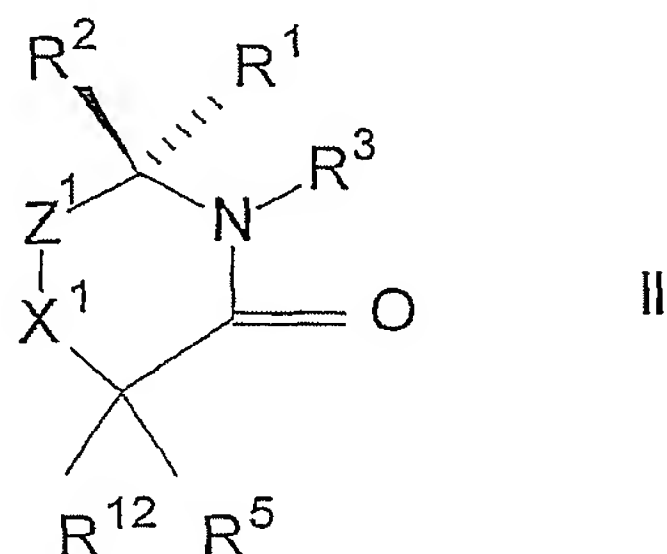
Examples of turn mimics and their modifications can be found in the following reviews: Hanessian et al, TETRAHEDRON 53: 12789-12854 SEP 22 1997; Gillespie et al, BIOPOLYMERS 43: 191-217 1997; and Burgess et al., ACCOUNTS CHEM RES 34: 826-835 2001). Recent examples of primary reports  
25        on turns include the following (and references therein) Maier et al, EUR J ORG CHEM: 2686-2689, 2002; Reid et al, J AM CHEM SOC 124: 5673-5683, 2002; Mahadevan et al, J BIOMOL STRUCT DYN 19: 775-788 2002; Eguchi et al, J MED CHEM 45: 1395-1398 2002; De Borggraeve et al, TETRAHEDRON LETTERS 42: 5693-5695 2001; Kohn et al, TETRAHEDRON LETT 42: 4453-  
30        4457 2001; Eguchi et al, TETRAHEDRON LETT 42: 1237-1239 2001; Manzoni et al, TETRAHEDRON 57: 249-255 2001; Jiang et al., HELV CHIM ACTA 83: 3097-3112 2000; Derrer et al, J CHEM SOC PERK T 1: 2957-2967 2000; Belvisi et al,



EUR J ORG CHEM: 2563-2569 2000; Claridge et al, BIOORG MED CHEM LETT  
6: 485-490 1996.

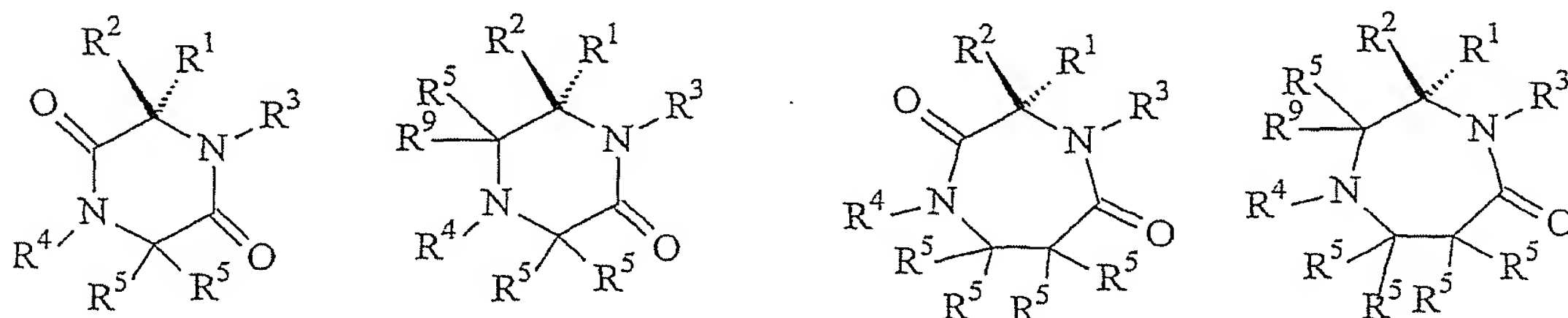
These include compounds of the general formula:

5

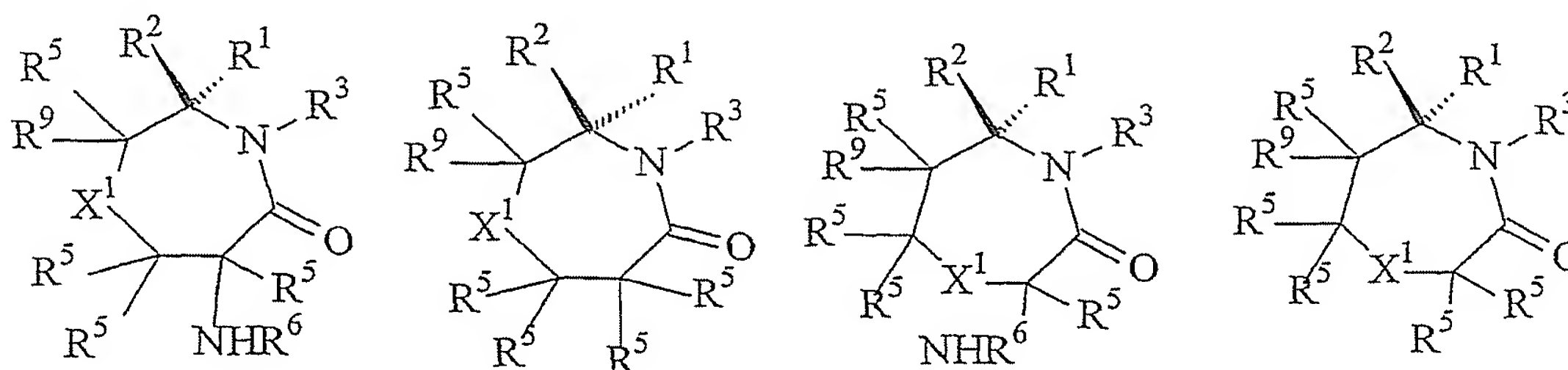


wherein  $R^1$  is such that it can form an electrostatic or H-bonding interaction with  
Gln-237 and or Arg-238, preferably  $CR^8R^9CONH_2$  or an analogue thereof where  $R^8$   
is hydrogen or a peptide or peptide mimetic (such as those composed of  $\beta$ -amino  
10 acids or peptide isosteres), and  $R^9$  is hydrogen, optionally functionalised alkyl,  
optionally functionalised aryl, heteroaryl or any combination thereof such as  
 $CH_2CONH_2$ ,  $R^2$  is hydrogen or a group that will interact favourably with Tyr-102 of  
FIH,  $R^3$  is H or a group which can form a H-bond with Asp-201,  $Z^1$  is  $>C=O$  or  
 $>CR^5R^9$  where  $R^5$  is hydrogen, optionally functionalised alkyl, aryl, or heteroaryl or  
15 any combination thereof,  $R^{12}$  is as defined for  $R^5$  or is  $NHR^6$  where  $R^6$  is  $COR^5$  or  
 $SO_2R^5$  and  $X^1$  is  $NR^4$ ,  $NR^4C(R^5)_2$ ,  $C(R^5)_2NR^4$ , or O or NH where  $R^4$  is  $COR^5$  or  
 $SO_2R^5$ . In this and in the other formulae each  $R^1, R^2, R^3, R^4, R^5, R^6, R^7, R^8, R^9, R^{10},$   
 $R^{11}$  and  $R^{12}$  can be the same or different. In particular, these compounds may have  
one of the formulae

20

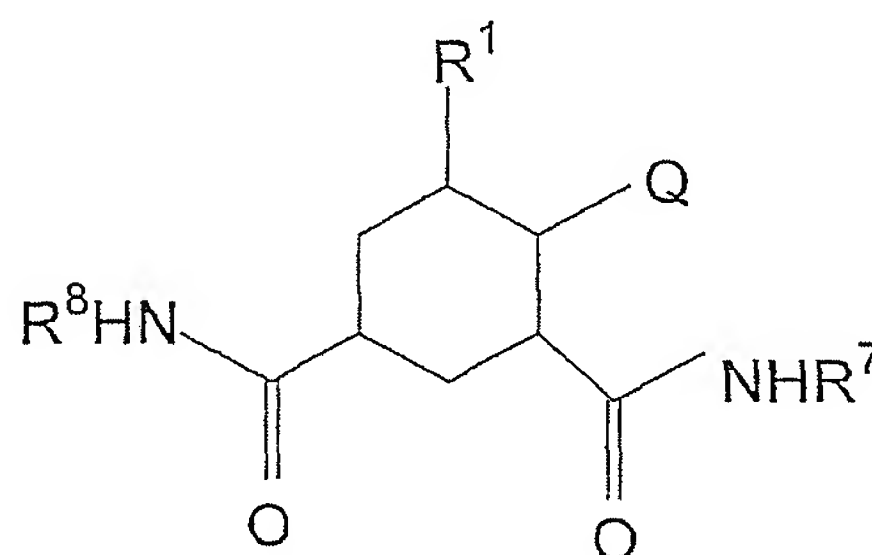


15



wherein the radicals are as defined above, and  $R^7$  and  $R^8$  are independently peptides or peptides mimetics or part peptide mimetics, such as those containing or consisting of beta-amino acid residues, urethane, sulphonamide or phosphonamide links.

Other compounds which can be used are those possessing the formula

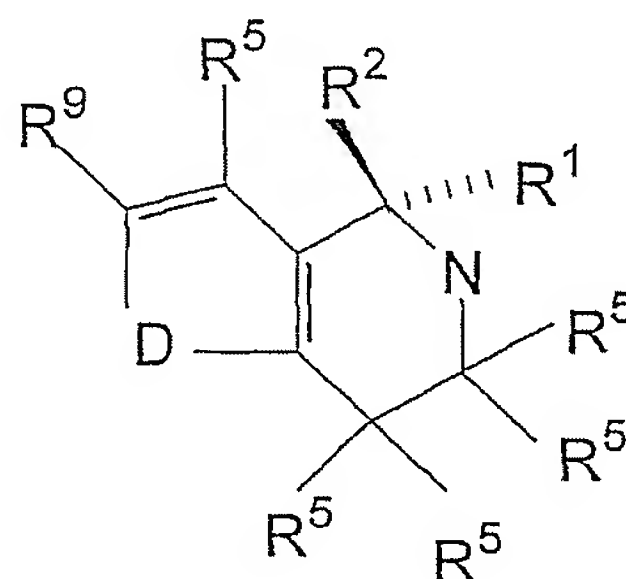


III

10

where  $Q$  represents H or OH and  $R^7$  and  $R^8$  are as defined above.

Further compounds which can be used possess the formula



IV

wherein  $R^1$ ,  $R^2$ ,  $R^5$  and  $R^9$  are as defined above and D is S, O, NH or  $CHR^9=CHR^9$ . Thus the ring attached to the six-membered ring is either a five-membered heterocyclic ring or an aryl ring.

In these formulae  $R^8$  and  $R^9$  can be optimised to bind in the channel linking the 2OG and peptide substrate binding sites and to the 2OG binding site itself.

Cyclic peptides acting as mimics of the turn adopted by CAD in site 1. The cyclo may be formed via peptide links, disulphide bonds or C-C bonds.

#### Inhibitors employing a combination of binding sites

It is well known that enzyme inhibitors competing for binding at more than one substrate or cosubstrate binding site, sometimes termed bisubstrate inhibitors, can be useful. Examples can be found in Wang et al, BIOCHEMISTRY-US: 15676-15683 2001; and Lerner et al, ANGEW CHEM INT EDIT 40, 4040-4041, 2001.

In the case of FIH and other 2OG oxygenases bisubstrate inhibitors may be useful since features of 2OG binding may be present in more than one enzyme whereas the CAD substrate is unique. Thus, inhibitors that bind to both binding sites may show improved selectivity over those that bind to the 2OG binding site only. The structural analyses enable the identification of such bisubstrate inhibitors. The 2OG and CAD binding sites are linked to each other via a 'channel' extending from the 2-oxo group of 2OG (or NOG) to the beta-carbon Asn-803 in the FIH.Fe.2OG/NOG.HIF(CAD) complexes. In the structures this 'channel' either appears empty but may be occupied by water molecules. The distance from the C of the 2-oxo group of 2OG to the beta-C of Asn-803 is ca. 6 Å. The distance from the 3-C of 2OG to the beta-C of Asn-803 is ca. 6.6 Å. The information from the structural analyses enables the identification of bisubstrate inhibitors, including the following:

These are compounds of formulae (II) to (IV) as defined above except that they are modified such that they can also bind into the 2OG binding pocket as defined by the crystallographic information. Thus, either  $R^2$  or  $R^1$  is modified such that they can bind into the 2OG binding pocket. The modification takes the form such that the general formula of  $R^1$  or  $R^2$  is A-X where X is as defined above and A links X to (II). A is of appropriate length such that X can bind to formula 1 the residues of the 5-

carboxylate of 2OG as discussed above under the heading Inhibitors Exploiting the 2OG binding sites.

More generally bi-substrate inhibitors of FIH can have the formula:



where X is as defined above, B is a linker group and C is an entity binding to part of the CAD binding site of FIH, in general CONH<sub>2</sub>.

B is typically a polymethylene group, generally having 6 to 8 carbon atoms or  
10 an equivalent group where one or more of the carbon atoms is replaced by a heteroatom, notably O, S or N and can be functionalised, for example with thiol, alcohol, carboxylate, hydroxamic acid or oxalate to mediate Fe binding. It is preferably 6 to 8 carbon atoms long or its equivalent. Alternatively, B is a linking group which possesses a ring, preferably of 5 to 7 members to which C is attached.

15

#### Inhibitors that bind to the 2OG binding site or part thereof and the peptide substrate

Another class of inhibitors bind to the enzyme-substrate complex, i.e. to FIH.Fe(II).HIF(CAD). The structural analyses enable the identification of such inhibitors. As described above 2OG and CAD binding sites are linked to each other  
20 via a 'channel' extending from the 2-oxo group of 2OG (or NOG) to the beta-carbon of Asn-803 in the FIH.Fe.2OG/NOG.HIF(CAD) complexes.

Inhibitors of this type may be defined as X-[B]-[E] where X is as defined above, B is a linker group such as defined above and E is an entity binding to part of the CAD when bound to HIF. E may bind to the backbone carbonyl oxygen of Asn-  
25 803 of CAD and to the NH<sub>2</sub> group of the primary amide of Asn-803.

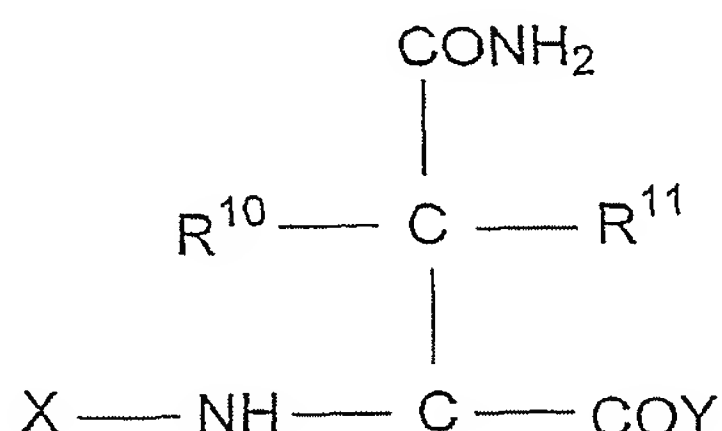
#### Mechanism based inhibitors

Another class of inhibitors is based upon substrate analogues that can undergo part of the catalytic cycle but either stall at an intermediate stage or cause an aberrant  
30 reaction resulting in damage or inhibition. The observation that FIH catalyses hydroxylation of Asn-803 at the beta-position together with the structural analyses enables the design of such inhibitors. Such compounds include analogues of the



substrates (inhibitors) in which Asn-803 is replaced with an analogue which does not undergo oxidation such as beta-fluoro- asparagine, beta-di-fluoro- asparagine, beta-methyl- asparagine, beta-dimethyl- asparagine derivatives. Alternatively derivatives that undergo oxidation to give an agent that can be oxidised to give an inactivating group such as an epoxide or metal chelating group may prepared (such mechanism based inhibitors are sometimes referred to as suicide inhibitors). In the case of FIH they include alpha-beta-dehydroasparagine and beta-methylene asparagine.

These include a compound having the formula



10

wherein X represents a valine residue or an analogue thereof and Y represents an alanine residue or an analogue thereof,  $\text{R}^{10}$  is fluorine or  $\text{C}_1 - \text{C}_3$  alkyl, especially methyl, and  $\text{R}^{11}$  is fluorine,  $\text{C}_1 - \text{C}_3$  alkyl or hydrogen i.e. the specified residue is  $\beta$ -mono- or di-fluoroasparagine or  $\beta$ -mono- or di-methylasparagine.

15

Alternatively, the compound above may be desaturated, i.e. is an alpha/beta dehydroamino acid ( $\text{R}^{11}$  not present) or  $\text{R}^{10}$  and  $\text{R}^{11}$  may be replaced by a methylene group, i.e. the residue is  $\alpha$ ,  $\beta$ -dehydro-asparagine or  $\beta$ -methylene asparagine.

20

If desired the valine residue is connected to one or more units of the peptide DESGLPQLTSYDCE - in the order given e.g. to glutamic acid (E) alone or to, for aspartic acid (D) - cysteine (C) - glutamic acid (E)-, or a longer chain such as PQLTSYDCE -.

25

For the compounds of this invention suitable aryl rings include phenyl and naphthalenyl, which may be further functionalised or fused to other ring systems. Suitable heterocyclic rings include thiophene, pyridine, quinoline, isoquinoline, pyrimidine, pyrazine, pyrone, chromone, coumarin, indole, isoindole, indolizine, benzofuran, pyridazine, purine, oxazole, pyrazole, isothiazole, pyrrolidine,

piperidine, indoline, benzothiaphen, morpholine, benzimidazole, azepine, azacine, azoine, oxepine, oxocine, oxoine, piperazine, oxazine, thiazine, thiepine, thiocine, thioine, furan, imidazole, azole, diazole, triazole and tetrazole ring systems that may be functionalised or fused to other ring systems.

5           The said alkyl and aryl groups and chains are typically functionalised by alcohol, fluorine, thiol, a carboxylic acid, phosphonic or phosphinic acid, sulphonic acid or other chelating group, in the case of the chains typically via an alkyl group. In the formulae described herein, a branched or straight C<sub>1</sub> to C<sub>6</sub> alkyl chain may be a methyl, ethyl, propyl, butyl, iso-butyl, *tert*-butyl, pentyl, neopentyl, *tert*-pentyl or a  
10       primary, secondary or tertiary hexyl group. Preferably the alkyl groups are methyl, the preferred heterocyclic rings are pyrrolidine and tetrahydropyran and the preferred aromatic rings are benzene, naphthalene and pyridine.

          The compounds which are acids can be present in the form of salts, such as sodium salts.

15           The crystal structure of FIH also allows identification of those residues involved in asparaginyl hydroxylase activity of FIH. The crystal structures may therefore be used to design modified FIH, for example, which has reduced or no asparaginyl hydroxylase activity, for example, by mutation of critical residue within the active site. In the alternative, those residues involved in substrate binding can be  
20       identified and modified, for example, to allow the asparaginyl hydroxylase to accept other substrates than HIF. For example, by enlarging or decreasing the asparagine binding pocket. Such modified asparaginyl hydroxylases can then be produced using standard techniques. The expected activity can then be assayed as described in more detail below, for example, to identify whether the hydroxylase activity with respect  
25       to HIF has been reduced or removed, or alternatively, to assess the asparaginyl activity or binding in respect to other substrates.

          Compounds which have been identified in accordance with the present invention can be further analysed in assays to monitor for activity of the asparagine hydroxylase enzyme directly. Agents which inhibit or reduce HIF asparagine  
30       hydroxylase activity reduce hydroxylation of HIF- $\alpha$  and lead to an increase in the interaction with P300 and in particular the CH1 domain and thus transcriptional activation. This in turn will lead to the activation of systemic local defences against

hypoxia or ischaemia that may include the promotion of angiogenesis, erythropoiesis, energy metabolism, inflammation, vasomotor function and will also affect apoptotic/proliferative responses.

We describe below in more detail a number of different assays that may be carried out to assay the activity of modulators of HIF hydroxylase activity or of FIH identified in accordance with the present invention and in particular of asparagine hydroxylase activity, or which affect regulation of HIF- $\alpha$  interaction with p300 in a cell and hence which affect HIF mediated activity. Some of these assays utilise HIF polypeptides, and HIF asparagine hydroxylases. Typically, the assays may utilise a human HIF asparagine hydroxylase such as FIH or a fragment or variant of a human HIF asparagine hydroxylase. These components are described in more detail below. Each of these components, where required, may be provided either in purified or unpurified form, for example, as cellular extracts or by purification of the relevant component from such extracts. Alternatively, the relevant component can be expressed using recombinant expression techniques and purified for use in the assay. Alternatively, the components may be expressed recombinantly in a cell for use in cell based assays.

Typically, a polynucleotide encoding the relevant component is provided within an expression vector. Such expression vectors are routinely constructed in the art and may for example involve the use of plasmid DNA and appropriate initiators, promoters, enhancers and other elements, such as for example polyadenylation signals which may be necessary and which are positioned in the correct orientation in order to allow full protein expression. Suitable vectors would be very readily apparent to those of skill in the art, such as those described in more detail herein with reference to the HIF hydroxylases. Promoter sequences may be inducible or constitutive promoters depending on the selected assay format. The promoter may be tissue specific. Examples of promoters and other flanking sequences for use in the expression vectors are described in more detail herein with reference to the HIF hydroxylases of the invention and in particular to the human HIF hydroxylases.

### HIF Polypeptides and Peptide Analogues

The assays of the present invention may use a substrate of a HIF asparagine hydroxylase and in particular an asparagine containing substrate of the enzyme. In particular, such substrates may be used in assays to monitor for the activity of a modulator of HIF asparagine hydroxylase activity. The substrate may be a HIF polypeptide or peptide analogue thereof. Typically, a HIF polypeptide will be used as the substrate.

Any suitable substrate in which an asparagine residue is hydroxylated by a FIH may be used. In preferred embodiments of the invention, such a substrate is a HIF polypeptide such as a HIF-1 $\alpha$  or HIF-2 $\alpha$  subunit protein or fragment of either or peptide analogue of the subunit or fragment. Preferably, the HIF- $\alpha$  peptide conveys an oxygen regulated response. Preferably, the HIF- $\alpha$  peptide has a CAD domain and is capable of oxygen regulated interaction with p300 and downstream transcriptional activation. Preferably, such HIF- $\alpha$  peptides are capable of interacting with the p300 CH1 domain. Preferably, such HIF polypeptides, fragments or peptide analogues incorporate an asparagine residue equivalent to Asn 803 defined with reference to HIF-1 $\alpha$ . The asparagine equivalent to Asn 803 of HIF-1 $\alpha$  may be determined by aligning the HIF variant, fragment or analogue to the sequence of HIF-1 $\alpha$  to obtain the best sequence alignment and identifying thereby the asparagine equivalent to Asn 803 of HIF-1 $\alpha$ .

A HIF polypeptide may be of eukaryotic origin, in particular a human or other mammalian, HIF- $\alpha$  subunit protein or fragment thereof. Alternatively, the polypeptide may be of *C. elegans* origin. In those assays which monitor for hydroxylation of HIF- $\alpha$  through its interaction with p300, the HIF polypeptide has the ability to bind to a wild type full length p300 protein or a fragment thereof comprising the CH1 domain. Preferably, such binding is able, in a hypoxic cellular environment, to activate transcription.

A number of HIF $\alpha$  subunit proteins have been cloned. These include HIF-1 $\alpha$ , the sequence of which is available as Genbank accession number U22431, HIF-2 $\alpha$ , available as Genbank accession number U81984 and HIF-3 $\alpha$ , available as Genbank accession numbers AC007193 and AC079154. These are all human HIF  $\alpha$  subunit proteins and all may be used in the invention. HIF- $\alpha$  subunit proteins from



other species, including murine HIF-1 $\alpha$  (accession numbers AF003695, U59496 and X95580), rat HIF-1 $\alpha$  (accession number Y09507), murine HIF-2 $\alpha$  (accession numbers U81983 and D89787) and murine HIF-3 $\alpha$  (accession number AF060194) may also be used in the invention.

5           One HIF- $\alpha$  protein of particular interest is the *C.elegans* HIF- $\alpha$  subunit protein. The *C.elegans* system may be used in assays of the present invention.

          There are a number of common structural features found in the two HIF- $\alpha$  subunit proteins identified to date. Some of these features are identified in O'Rourke *et al* (1999, J. Biol. Chem., 274; 2060-2071) and may be involved in the trans-  
10   activation functions of the HIF- $\alpha$  subunit proteins. One or more of these common structural features are preferred features of the HIF polypeptides.

          Variants of the above HIF- $\alpha$  subunits may be used, such as synthetic variants which have at least 45% amino acid identity to a naturally occurring HIF- $\alpha$  subunit (particularly to a human HIF- $\alpha$  subunit such as, for example HIF-1 $\alpha$ ), preferably at  
15   least 50%, 60%, 70%, 80%, 90%, 95% or 98% identity. Such variants may include substitutions or modifications as described above with respect to HIF hydroxylases. Amino acid activity may also be calculated as described above with reference to HIF hydroxylases.

          HIF fragments may also include non-peptidyl functionalities and may be  
20   optimised for assay purposes such that the level of identity is lowered. Such functionalities may be covalently bound such as sugars or non-covalently bound such as metal ions.

          HIF $\alpha$  polypeptides as described herein may be fragments of the HIF- $\alpha$  subunit protein or variants as described above, provided that said fragments retain the  
25   ability to interact with a wild-type p300 CH1 domain. When using proteinogenic amino acid residues, such fragments are desirably at least 20, preferably at least 40, 50, 75, 100, 200, 250 or 400 amino acids in size. Desirably, such fragments include asparagine 803.

          Cell based assays of the present invention may involve upregulation of an  
30   endogenous HIF- $\alpha$  or expression of a HIF- $\alpha$  by recombinant techniques and in particular of HIF-1 $\alpha$ .



### Assay Methods

The present invention provides an assay method for an agent identified as a modulator of asparagine hydroxylation of hypoxia inducible factor. The method comprises contacting a HIF asparagine hydroxylase and a test substance in the presence of a substrate of the hydroxylase under conditions in which asparagine hydroxylation occurs in the absence of the test substrate and determining asparagine hydroxylation of the substrate. In an alternative assay, HIF asparagine hydroxylase and the test substance are contacted in the presence of the substrate of the hydroxylase under conditions in which hydroxylation does not occur in the absence of the test substrate. Determination of any asparagine hydroxylation is monitored to identify whether the agent actively acts as a promoter of asparagine hydroxylase.

FIH has been found to hydroxylate HIF- $\alpha$  at an asparagine residue within the CAD domain. This hydroxylation mediates p300 binding and in particular, reduces p300 binding. Such binding leads to transcriptional activation. This interaction and activation may also be used as the basis for an assay of the invention.

Such assays of the present invention may be used to assay the activity of inhibitors of HIF asparagine hydroxylase activity and are thus preferably carried out under conditions under which asparagine hydroxylation would take place in the absence of the test substance. The assays of the invention may also be used to assay the activity of inhibitors which are specific for HIF asparagine hydroxylases and which do not have activity or are less active with other hydroxylases, for example, such as HIF prolyl hydroxylases or other asparagine/aspartamic acid hydroxylases. The assays of the invention may also be used to assay the activity of hydroxylase modulators, such as HIF prolyl hydroxylase inhibitors which are not expected to have activity on FIH based on structural modelling studies, and hence may be used to identify inhibitors which are specific for prolyl hydroxylase.

### Methods for monitoring modulation

The precise format of any of the screening or assay methods of the present invention may be varied by those of skill in the art using routine skill and knowledge. The skilled person is well aware of the need to additionally employ appropriate controlled experiments. The assays of the present invention may involve monitoring

for asparagine hydroxylation of a suitable substrate, monitoring for the utilisation of substrates and co-substrates, monitoring for the production of the expected products between the enzyme and its substrate. Assay methods of the present invention may also involve screening for the direct interaction between components in the system.

5 Alternatively, assays may be carried out which monitor for downstream effects such as binding of HIF by p300 and downstream effects mediated by HIF such as HIF mediated transcription using suitable reporter constructs or by monitoring for the upregulation of genes or alterations in the expression patterns of genes known to be regulated directly or indirectly by HIF.

10 Various methods for determining hydroxylation are known in the art and are described and exemplified herein. Any suitable method may be used for determining activity of the HIF hydroxylase such as by substrate or co-substrate utilization, product appearance such as peptide hydroxylation or down-stream effects mediated by hydroxylated or non-hydroxylated products.

15 Assays may be carried out to monitor directly for hydroxylation of the relevant asparagine residue or another position. Alternatively, assays may be carried out to monitor for depletion of co-factors and co-substrates. Alternatively, such assays may monitor the downstream effects of hydroxylation of HIF or indeed inhibition of hydroxylation of HIF, for example, by monitoring the interaction  
20 between HIF and p300 or HIF mediated transcription. Alternatively, reporter gene constructs driven by HIF regulated promoters may be used. Assays are also provided for the identification of enhancers of the activity of the HIF asparagine hydroxylase. Such enhancers may be used to reduce HIF $\alpha$  activity.

In one embodiment, a suitable substrate of the HIF asparagine hydroxylase is  
25 provided. This may be HIF- $\alpha$  or a fragment thereof which includes a CAD domain or which includes a residue equivalent to Asn 803 of HIF-1 $\alpha$ . The substrate may not be initially hydroxylated at the Asn 803 position. This may be achieved by providing synthetic polypeptide substrates, or by producing HIF- $\alpha$  polypeptides in bacterial cells, insect cells or mammalian cells or in *in vitro* transcription and translation  
30 systems. Alternatively, assays may be carried out over a selected time course such that the substrate is produced during the course of the assay, initially in un-hydroxylated form.

The substrate, enzyme and potential inhibitor compound may be incubated together under conditions which, in the absence of inhibitor provide for hydroxylation of Asn 803, and the effect of the inhibitor may be determined by determining hydroxylation of the substrate. This may be accomplished by any  
5 suitable means. Small polypeptide substrates may be recovered and subject to physical analysis, such as mass spectrometry or chromatography, or to functional analysis, such as the ability to bind to p300 (or displace a reporter molecule from p300). Such methods are known as such in the art and may be practiced using routine skill and knowledge. Determination may be quantitative or qualitative. In  
10 both cases, but particularly in the latter, qualitative determination may be carried out in comparison to a suitable control, e.g. a substrate incubated without the potential inhibitor.

Inhibitor compounds which are identified in this manner may be recovered and formulated as pharmaceutical compositions.

15 Assays in accordance with the present invention may involve monitoring for the interaction between p300 and HIF. The interaction between HIF and p300 is mediated by hydroxylation of HIF. Transcription and expression of genes known to be upregulated or down regulated by the presence of HIF could be monitored. In particular, upregulation of HIF regulated genes would demonstrate inhibition of  
20 asparagine hydroxylation whereas down regulation would suggest enhancement or promotion of asparagine hydroxylation.

In alternative embodiments, reporter constructs may be provided in which promoters mediated by HIF are provided operably linked to a reporter gene. Any suitable reporter gene could be used, such as for example enzymes which may then  
25 be used in colorimetric, fluorometric, fluorescence resonance or spectrometric assays.

HIF asparagine hydroxylase is a 2OG dependent oxygenase. In the assay methods described herein, typically the HIF asparagine hydroxylase and the substrate of the hydroxylase are contacted in the presence of a co-substrate, such as 2-oxoglutarate (2OG). The hydroxylase activity of the HIF hydroxylase may be  
30 determined by determining the turnover of the co-substrate. This may be achieved by determining the presence and/or amount of reaction products, such as hydroxylated

substrate or succinic acid. The amount of product may be determined relative to the amount of substrate. Typically, in such embodiments the substrate may be an HIF- $\alpha$  polypeptide and, for example, the product measured may be hydroxylated HIF- $\alpha$  polypeptide.

5           Alternatively, the end-point determination may be based on conversion of HIF $\alpha$  or peptide fragments (including synthetic and recombinant peptides) derived from HIF $\alpha$  into detectable products. Peptides may be modified to facilitate the assays so that they can be rapidly carried out and may be suitable for high throughput screening.

10           For example, reverse phase HPLC (C-18 octadecylsilane column), may be used to separate starting synthetic peptide substrates for HIF hydroxylase from the asparagine hydroxylated products, as the latter have a shorter retention time in the column. Modifications of this assay or alternative assays for HIF hydroxylase activity may employ, for example, mass spectrometric, spectroscopic, and/or  
15           fluorescence techniques as are well known in the art (Masimirembwa C. *et al* Combinatorial Chemistry & High Throughput Screening (2001) 4 (3) 245-263, Owicki J. (2000) J. Biomol. Screen. 5 (5) 297-305, Gershkovich A *et al* (1996) J. Biochem. & Biophys. Meths. 33 (3) 135-162, Kraaft G. *et al* (1994) Meths. Enzymol. 241 70-86). Fluorescent techniques may employ versions of the substrate  
20           modified in such as way as to carry out or optimise spectroscopic or fluorescence assays.

            For example, HIF $\alpha$  polypeptide may be immobilised e.g. on a bead or plate, and hydroxylation of the appropriate residue detected using an antibody or other binding molecule which binds the CAD binding domain of HIF $\alpha$  with a different  
25           affinity when an asparagine 803 is hydroxylated from when the residue is not hydroxylated. Such antibodies may be obtained by means of standard techniques which are well known in the art, e.g. using a hydroxylated HIF $\alpha$  peptide.

            Binding of a molecule which discriminates between the hydroxylated and non-hydroxylated form of a HIF $\alpha$  polypeptide may be assessed using any technique  
30           available to those skilled in the art, which may involve determination of the presence of a suitable label.



Assay methods of the present invention may also take the form of an *in vivo* assay. The *in vivo* assay may be performed in a cell line such as a yeast strain in which the relevant polypeptides or peptides are expressed from one or more vectors introduced into the cell.

5

#### In vivo assays

The assays may be carried out using cell based, organ based or whole animal assays conducted *in vivo*. Such assays may utilize the endogenous expression of the HIF hydroxylase nucleotides and/or polypeptides. In other forms of the invention, upregulation of specific endogenous HIF hydroxylases may be achieved by  
10 stimulators of the expression thereof. Such stimulators may be growth factors or chemicals that upregulate specific HIF asparagine hydroxylases. In another form of the assay, nucleotide constructs may be introduced into cells or transgenic animals to increase production of one or more specific HIF asparagine hydroxylases.

15 HIF complexed with p300 activate hypoxia response elements that are found in the promoters and/or enhancers of endogenous genes that are regulated by the said HIF complexes. Such hypoxia response elements may also be isolated and operationally linked to reporter genes so as to assay the activity of the HIF complex through detection and/or quantitation of the reporter gene or its product. Therefore in  
20 a further form of the invention the activity of a HIF- $\alpha$  polypeptide that is regulated by HIF asparagine hydroxylase will be assayed by measuring the effects of the HIF complex on the expression of an endogenous gene or reporter gene that is functionally linked to a HIF binding hypoxia response element. Examples of endogenous genes that are regulated in this way are to be found in the role of the aryl  
25 hydrocarbon nuclear translocator (ARNT) in hypoxic induction of gene expression, see for example, Studies in ARNT-deficient cells. S.M. Wood, J.M. Gleadle, C.W. Pugh, O. Hankinson, P.J. Ratcliffe. Journal of Biological Chemistry 271 (1996) 15117-15123, and Hypoxia inducible expression of tumor-associated carbonic anhydrases, C.C. Wykoff, N.J.P. Beasley, K.J. Turner, J. Pastorek, A. Sibtain. G.D.  
30 Wilson, H. Turley, K. Talks, P.H. Maxwell, C.W. Pugh, P.J. Ratcliffe, A.L. Harris. Cancer Research 60 (2000) 7075-7083. Examples include but are not limited to glucose transporter isoform 1, phosphoglycerate kinase-1, carbon anhydrase isoform



9, vascular endothelial growth factor. Each of said genes contains one or hypoxia response elements that may be isolated and operationally linked as single or multiple copies to a reporter gene for the measurement of activity of a HIF- $\alpha$  polypeptide that varies in accordance with the activity of a HIF hydroxylase.

5       The activity of genes or gene products that are regulated by a HIF- $\alpha$  polypeptide in accordance with the activity of a HIF hydroxylase affects cellular, organ, and animal physiology. Assays that utilise a specific functional response that is regulated in accordance with the activity of a HIF- $\alpha$  polypeptide in accordance with the activity of a HIF hydroxylase may be used. Such responses include the  
10 uptake rate of glucose or glucose analogues that are not metabolized, the growth of blood vessels by angiogenesis, the activity of a carbonic anhydrase enzyme. It is recognised that many other responses that operate at a cellular or systemic level are controlled by the activity of a HIF- $\alpha$  polypeptide in accordance with the activity of a HIF hydroxylase and may be utilized as assays of the said HIF hydroxylase activity  
15 in further aspects of the invention.

A HIF- $\alpha$  polypeptide that is a substrate for a HIF hydroxylase may be fused to a further polypeptide so as to cause the activity of the said HIF hydroxylase to regulate the activity of the fusion peptide. Accordingly a further form of the invention provides for the assay of the activity of a fusion polypeptide. In the  
20 preferred form such a fusion polypeptide may contain the whole or part of a HIF- $\alpha$  polypeptide, particularly including Asn 803, or the CAD domain. The Gal4 DNA binding domain including the amino acids 1-143 together with the Gal binding upstream activating sequence (UAS) is an example of such a transcription factor and cognate DNA response element whose operation can be assayed by those skilled in  
25 the art.

### Selectivity

It may also be advantageous to modulate HIF asparagine hydroxylase selectively, as a single target, or in selected hydroxylase groups as well as an entire  
30 family. Agents which modulate HIF asparagine hydroxylase activity are therefore preferably specific i.e. they have an increased or enhanced effect on a HIF asparagine hydroxylase relative to other 2OG dependent oxygenases.

Assay methods as described herein may therefore further comprise contacting the test compound with one or more 2OG dependent oxygenases under conditions in which said 2OG dependent oxygenases are normally active and determining activity of said oxygenases. A difference in activity in the presence relative to the absence of test compound is indicative of the test compound modulating the activity of the one or more 2OG dependent oxygenases.

A test compound which provides increased or enhanced modulation of a HIF asparagine hydroxylase, relative to the one or more 2OG dependent oxygenases shows selectivity or specificity for the HIF hydroxylase.

2OG dependent oxygenases may include for example, clavaminte synthase, Alk B deacetoxycephalosporin C synthase, collagen-prolyl-4-hydroxylase, collagen prolyl-3-hydroxylase, lysyl hydroxylase, aspartyl hydroxylase, phytanoyl coenzyme A hydroxylase or gamma-butyrobetaine hydroxylase. 2OG dependent oxygenases may be mammalian, preferably human polypeptides.

The invention provides for the use of such selective inhibitors of HIF asparagine hydroxylases in the manufacture of a medicament for the treatment of a condition associated with reduced HIF activity.

#### Therapeutic Applications

A compound, substance or agent which is found to have the ability to affect the hydroxylase activity of a HIF asparagine hydroxylase, or the compounds referred to herein as FIH inhibitors has therapeutic and other potential in a number of contexts. For therapeutic treatment, such a compound may be used in combination with any other active substance, e.g. for anti-tumour therapy another anti-tumour compound or therapy, such as radiotherapy or chemotherapy.

An agent identified using one or more primary screens (e.g. in a cell-free system) as having ability to modulate the HIF $\alpha$  asparagine hydroxylation activity of a HIF hydroxylase may be assessed further using one or more secondary screens. A secondary screen may involve testing for an increase or decrease in the amount of HIF- $\alpha$  or HIF activity, for example as manifest by the level of a HIF target gene or process present in a cell in the presence of the agent relative to the absence of the agent.

A HIF hydroxylase or a HIF polypeptide may be used in therapies which include treatment with full length polypeptides or fragments thereof, or otherwise modified polypeptides (e.g. to enhance stability or ensure targeting, including in conjunction with other active agents such as antibodies. For example, mutation of  
5 HIF-1 $\alpha$  to replace Asn 803 with another amino acid residue may prevent hydroxylation and thus promote interaction of HIF- $\alpha$  with p300 and stimulate transcriptional activation.

Generally, an agent, compound or substance which is a modulator according to the present invention is provided in an isolated and/or purified form, i.e.  
10 substantially pure. This may include being in a composition where it represents at least about 90% active ingredient, more preferably at least about 95%, more preferably at least about 98%. Any such composition may, however, include inert carrier materials or other pharmaceutically and physiologically acceptable excipients, such as those required for correct delivery, release and/or stabilisation of the active  
15 agent. Typically, the concentration in such compositions is 0.1 to 50%, generally 0.5 to 20%, especially 1 to 10% by weight based on the weight of the composition. As noted below, a composition according to the present invention may include in addition to an modulator compound as disclosed, one or more other molecules of therapeutic use, such as an anti-tumour agent.

20

#### Products obtained by assays of the invention

The invention further provides compounds obtained or identified by methods of the present invention, and compositions comprising said compounds, such as pharmaceutical compositions wherein the compound is in a mixture with a  
25 pharmaceutically acceptable carrier or diluent. The carrier may be liquid, e.g. saline, ethanol, glycerol and mixtures thereof, or solid, e.g. in the form of a tablet, or in a semi-solid form such as a gel formulated as a depot formulation or in a transdermally administerable vehicle, such as a transdermal patch.

The invention further provides a method of treatment which includes  
30 administering to a patient an agent which interferes with the hydroxylation of the asparagine target residue of an HIF $\alpha$  polypeptide by a HIF hydroxylase. Such agents may include inhibitors of asparagine hydroxylase activity. The invention also

provides a method of treatment which includes administering to a patient a compound as defined above.

- The therapeutic/prophylactic purpose may be related to the treatment of a condition associated with reduced or suboptimal or increased HIF levels or activity, or conditions in which have normal HIF levels, but where an modulation in HIF activity such as an increase or decrease in HIF activity is desirable such as:
- (i) ischaemic conditions, for example organ ischaemia, including coronary, cerebrovascular and peripheral vascular insufficiency. The therapy may be applied in two ways; following declared tissue damage, e.g. myocardial infarction (in order to limit tissue damage), or prophylactically to prevent ischaemia, e.g. promotion of coronary collaterals in the treatment of angina.
  - (ii) wound healing and organ regeneration
  - (iii) auto-, allo-, and xeno- transplantation.
  - (iv) systemic blood pressure
  - (v) cancer; HIF $\alpha$  is commonly up-regulated in tumour cells and has major effects on tumour growth and angiogenesis.
  - (vi) inflammatory disorders.
  - (vii) pulmonary arterial blood pressure, neurodegenerative disease.

Modulating HIF prolyl hydroxylase activity in a person, an organ, or a group of cells may be exploited in different ways to obtain a therapeutic benefit:

- (a) Non cell autonomous: The HIF system is used by cells to influence the production of substances which signal to other cells. These signals may then have effects at (i) a distant site (for example erythropoietin acts on the bone marrow) or (ii) locally (angiogenic growth factors increase the local formation of blood vessels). Manipulating non cell autonomous behaviour via altering hydroxylase activity is therefore useful in the treatment of anaemia, and local ischaemia, for example in the eye, brain, heart and limbs. Many other signals that are involved in aspects of physiological homeostasis may be, or are known to be, adjusted by HIF activation. Consequently altering HIF prolyl hydroxylase activity may be used to potentiate or initiate a helpful response for a therapeutic benefit, or to prevent or ameliorate a harmful response. For example, this approach can be used to alter appetite, or blood pressure in the systemic or pulmonary beds.



(b) Cell autonomous: the HIF system is also used by cells to regulate cellular metabolism, and decisions concerning differentiation, proliferation and apoptosis. Therefore manipulating the HIF system can be used to alter the viability and behaviour of cells. An increase in cell viability can be achieved by increasing HIF activation, for example in an ischaemic tissue. This approach can also be used in improving pancreatic beta cell viability as a way of ameliorating diabetes, or of improving the viability or function of a group or groups of neurons in Parkinson's disease, motorneurone disease or forms of dementia. In a different approach, the HIF signal can be manipulated to prevent a group of cells proliferating, or to promote its death or differentiation. For example transient activation of the HIF system in a malignant tumour can be used to provoke death of a substantial number of tumour cells.

#### Pharmaceutical Compositions

In various further aspects, the present invention thus provides a pharmaceutical composition, medicament, drug or other composition for such a purpose, the composition comprising one or more agents, compounds or substances as described herein, including HIF asparagine hydroxylase inhibitors, or one or more compounds of formula (A) to (F) or derivatives thereof, the use of such a composition in a method of medical treatment, a method comprising administration of such a composition to a patient, e.g. for treatment(which may include preventative treatment) of a medical condition as described above, use of such an agent compound or substance in the manufacture of a composition, medicament or drug for administration for any such purpose, e.g. for treatment of a condition as described herein, and a method of making a pharmaceutical composition comprising admixing such an agent, compound or substance with a pharmaceutically acceptable excipient, vehicle or carrier, and optionally other ingredients.

In one embodiment the method for providing a pharmaceutical composition may typically comprise:

- (a) identifying an agent in accordance with the invention; and
- (b) formulating the agent thus identified with a pharmaceutically acceptable excipient.



The agent may be used as sole active agent or in combination with one another or with any other active substance, e.g. for anti-tumour therapy another anti-tumour compound or therapy, such as radiotherapy or chemotherapy.

Whatever the agent used in a method of medical treatment of the present invention, administration is preferably in a "prophylactically effective amount" or a "therapeutically effective amount" (as the case may be, although prophylaxis may be considered therapy), this being sufficient to show benefit to the individual. The actual amount administered, and rate and time-course of administration, will depend on the nature and severity of what is being treated. Prescription of treatment, e.g. decisions on dosage etc, is within the responsibility of general practitioners and other medical doctors.

An agent or composition may be administered alone or in combination with other treatments, either simultaneously or sequentially dependent upon the condition to be treated, e.g. as described above.

Pharmaceutical compositions according to the present invention, and for use in accordance with the present invention, may include, in addition to active ingredient, a pharmaceutically acceptable excipient, carrier, buffer, stabiliser or other materials well known to those skilled in the art. In particular they may include a pharmaceutically acceptable excipient. Such materials should be non-toxic and should not interfere with the efficacy of the active ingredient. The precise nature of the carrier or other material will depend on the route of administration, which may be oral, or by injection, e.g. cutaneous, subcutaneous or intravenous. The compositions will typically be sterile.

Pharmaceutical compositions for oral administration may be in tablet, capsule, powder or liquid form. A tablet may include a solid carrier such as gelatin or an adjuvant. Liquid pharmaceutical compositions generally include a liquid carrier such as water, petroleum, animal or vegetable oils, mineral oil or synthetic oil. Physiological saline solution, dextrose or other saccharide solution or glycols such as ethylene glycol, propylene glycol or polyethylene glycol may be included.

For intravenous, cutaneous or subcutaneous injection, or injection at the site of affliction, the active ingredient will be in the form of a parenterally acceptable aqueous solution which is pyrogen-free and has suitable pH, isotonicity and stability.

Those of relevant skill in the art are well able to prepare suitable solutions using, for example, isotonic vehicles such as Sodium Chloride Injection, Ringer's Injection, Lactated Ringer's Injection. Preservatives, stabilisers, buffers, antioxidants and/or other additives may be included, as required.

5       Liposomes, particularly cationic liposomes, may be used in carrier formulations. Examples of techniques and protocols mentioned above can be found in Remington's Pharmaceutical Sciences, 16th edition, Osol, A. (ed), 1980.

      The substance or composition may be administered in a localised manner to a particular site or may be delivered in a manner in which it targets particular cells or  
10       tissues, for example using intra-arterial stent based delivery.

      Targeting therapies may be used to deliver the active substance more specifically to certain types of cell, by the use of targeting systems such as antibody or cell specific ligands. Targeting may be desirable for a variety of reasons, for example if the agent is unacceptably toxic, or if it would otherwise require too high a  
15       dosage, or if it would not otherwise be able to enter the target cells.

      In a further embodiment the invention provides for the use of an agent of the invention in the manufacture of a medicament for the treatment of a condition associated with increased or decreased HIF levels or activity. The condition may, for example, be selected from the group consisting of ischaemia, wound healing, auto-  
20       allo-, and xeno- transplantation, systemic high blood pressure, cancer, and inflammatory disorders.

### Examples

#### 25       **Example 1**

      The position on Asn803 of human HIF-1 $\alpha$  that is hydroxylated was identified as described in the following. cDNA sequences encoding FIH-1 were cloned into the pET28a(+) vector (from Novagen) to yield FIH-1 protein with an N-terminal His<sub>6</sub>tag to facilitate purification. Purification of crude material by nickel affinity  
30       chromatography, followed by thrombin cleavage of the His<sub>6</sub> tag, and size exclusion chromatography (Superdex S75) yielded >95% pure protein by SDS-PAGE analysis. Mass spectrometry confirmed the identity of the isolated species. The 19-residue

peptide comprising amino acids 788-806 of human HIF-1 $\alpha$  was modified by aerobic incubation with FIH-1 FIH (Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002) in the presence of ascorbate, DTT, catalase, 2-oxoglutarate, and iron(II) for 30 minutes at 37°C. The reaction was quenched by cooling to 4°C and addition of an equal volume of methanol. Precipitate was removed by centrifugation and the supernatant purified by HPLC using a Jupiter C4 column (15cm x 4.6mm). Peptide was eluted using a gradient of acetonitrile in 0.1% trifluoroacetic acid, freeze-dried from the HPLC solvent for amino acid and mass spectrometric analyses. The sample was freeze-dried a second time from D<sub>2</sub>O in preparation for NMR analysis.

Catalytic FIH-1 mediated hydroxylation of a synthetic 19 residue peptide corresponding to residues 788-806 of HIF-1 $\alpha$  was confirmed by mass spectrometric analysis of HPLC purified material: Native peptide 19mer  $[M+2H]^{2+} = 1026.67\text{Da}$ , modified peptide 19mer  $[M+2H]^{2+} = 1034.61\text{Da}$ , a mass difference of +8Da of the doubly charged ions, corresponding to +16Da in the peptide (oxygen). N-Terminal Edman degradation of the product peptide gave the following sequence: DESGLPQLTSYDCEVxA, where x was not asparagine. The peak from this (16th) cycle of Edman degradation ran to a similar position as the  $\beta$ -hydroxyasparagine standard. Acid hydrolysis of the modified peptide followed by amino acid analysis showed the presence of  $\beta$ -hydroxyaspartic acid only.

Both  $^1\text{H}$  and  $^{13}\text{C}$  chemical shift changes between the 19mer peptide substrate and the HPLC purified incubation product were assessed by 2D  $^1\text{H}$ - $^{13}\text{C}$  HSQC experiments. In the substrate a grouping of four  $\beta$ -CH<sub>2</sub> resonances were assigned as belonging to Asp-1, Tyr-11, Asp-12 and Asn-16 according to their  $^1\text{H}$  and  $^{13}\text{C}$  shifts (Evans, J. N. S. (1995) Biomolecular NMR Spectroscopy, Oxford University Press, Oxford, UK). In the product it was clear from both the 2D HSQC and the 1D proton spectra that only three of these four resonances are present. Comparison of the two spectra indicates that the signal assigned to the Asn-16  $\beta$ -carbon (at  $\delta\text{H}$  2.813 and 2.695ppm and  $\delta\text{C}$  37.40ppm in the substrate) has disappeared, consistent with hydroxylation of the asparagine residue at its  $\beta$ -carbon. The resonances due to the two aspartic acid residues had shifted slightly, presumably due to changes in the protonation state, and now occur at a similar  $^1\text{H}$  chemical shift as the  $\beta$ -protons of the

asparagine in the substrate. A difference in the oxidation state of the cysteine between the two samples is unlikely given the near identical chemical shifts for the cysteinyl  $\beta$ -carbon and hydrogens. The change from a double doublet to a single doublet for the  $\beta$ -hydrogen of the hydroxylated residue also rules out any possibility the observed alterations in the NMR spectrum are due to aggregation. Two new resonances have appeared in the product spectrum at  $\delta$ H 4.913 ppm and  $\delta$ C 56.26 ppm and at  $\delta$ H 4.654 ppm and  $\delta$ C 72.22 ppm. These resonances correlate with one another in the 2D COSY spectrum and share a  $^1\text{H}$ - $^1\text{H}$  coupling constant of 2.4 Hz and are therefore assigned as the  $\text{CH}^\alpha$ - $\text{CH}^\beta$  of the hydroxylated asparagine. The appearance of these resonances also coincides with the disappearance of the  $\delta$ H 4.706 ppm and  $\delta$ C 51.43 ppm resonances observed in the substrate spectra, which is therefore assigned as the  $\text{CH}^\alpha$  of the parent asparagine prior to modification. Comparison of the  $\text{CH}^\alpha$ - $\text{CH}^\beta$  coupling constant of 2.4 Hz observed for the hydroxylated Asn-803, with literature values implied the *threo* isomer is produced.

In summary of the above  $^1\text{H}$ -NMR experiments: The HSQC experiments gave direct evidence for hydroxylation occurring at the  $\beta$ -carbon of the target asparagine, with the hydroxylated  $\beta$ -carbon appearing significantly deshielded (at 72.22 ppm) and the adjacent  $\alpha$ -carbon deshielded to a lesser extent (at 56.26 ppm) relative to the parent asparagine. Changes of these magnitudes in the  $^{13}\text{C}$  chemical shifts are inconsistent with hydroxylation of the side-chain nitrogen, but consistent with hydroxylation at the  $\beta$ -carbon. Further, the  $^{13}\text{C}$  spectrum of free DL-*threo*- $\beta$ -hydroxyasparagine (this study), has resonances at 58.63 ppm and 73.85 ppm corresponding to  $\alpha$ - and  $\beta$ -carbons. The product assignment is also consistent with  $^1\text{H}$ -NMR chemical shifts of the  $\alpha$ - and  $\beta$ -hydrogens in the  $\beta$ -hydroxyaspartyl residues in EGF-like domains which are 4.48 ppm and 4.36 ppm respectively (with respect to water at 4.75 ppm) when calcium is absent (Selander et al, Biochemistry 29, 8111-8118). The analysis of the coupling constant reported here suggests that the *threo*-isomer is the one formed on hydroxylation of Asn-803 by FIH-1.

Two reports (Dames et al., (2002) *Proc. Natl. Acad. Sci. U. S. A.* 99, 52715276; Freedman et al, (2002) *Proc. Natl. Acad. Sci. U. S. A.* 99, 53675372) reveal how  $\beta$ -hydroxylation of Asn-803 of HIF-1 $\alpha$  would be damaging to complex formation with



p300. Although the position of hydroxylation was not identified in either report, both imply that hydroxylation at the *pro-S* position of the  $\beta$ -carbon, *i.e.* to give the *threo* (2*S*, 3*S*)-isomer, would interfere with the hydrogen bonding that maintains the  $\alpha$ -helical conformation adopted by this part of HIF-1 $\alpha$ , and also create a need for the energetically unfavourable desolvation of the hydroxyl group. A steric clash between the inserted *pro-S* hydroxyl group and Ile-353 (numbering from Dames *et al* (2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 52715276) of p300 would disrupt the interaction of the two proteins. Presumably the same mechanism is also used to abrogate the interaction of HIF-2 $\alpha$  and p300. The discovery that it is the beta-position of Asn-803 that is modified and the associated mechanistic implications may be used in the design of compounds that bind to p300 thereby displacing HIF-alpha and/in the design of inhibitors of FIH (see below); in both cases to enable pro-angiogenic pharmaceutical agents.

## 15 Example 2

To obtain an FIH:CAD complex suitable for X-ray analysis without oxidation of the CAD or the Fe<sup>(II)</sup>, FIH and various CAD fragments from seven to fifty-two residues were co-crystallised with Fe<sup>(II)</sup> and 2OG under anaerobic conditions. Structures were also obtained for FIH complexed with Fe<sup>(II)</sup> and *N*-oxaloylglycine (NOG, an FIH inhibitor), (anaerobically) and Zn<sup>(II)</sup> and NOG (aerobically). These structures were solved by molecular replacement using a model obtained by multiple anomalous dispersion on selenomethionine-substituted apo-FIH. Crystalline FIH:CAD complexes were obtained with CAD<sub>786-826</sub>, Fe<sup>(II)</sup> and NOG or 2OG (structures 1 and 2, Table 1), CAD<sub>775-826</sub> with Zn<sup>(II)</sup> and NOG (structure 3). Crystallisation attempts with CAD<sub>787-806</sub>, CAD<sub>850-862</sub> (HIF-2 $\alpha$ , equivalent to HIF-1 $\alpha$  CAD<sub>802-814</sub>) and CAD<sub>800-806</sub> did not result in FIH:CAD complexes; solution analyses indicated that CAD fragments shorter than twenty residues are not efficient *in vitro* substrates.



Table 1 Summary of FIH:CAD-fragment complex structures<sup>\*</sup>

| Structure No. | Resolution (Å) | Metal | Co-substrate | Co-crystallisation CAD peptide | Site 1 CAD residues resolved | Site 2 CAD residue resolved | R <sub>free</sub> (%) | R.m.s.d. from Struct. 1 (Å) | PDB ID. |
|---------------|----------------|-------|--------------|--------------------------------|------------------------------|-----------------------------|-----------------------|-----------------------------|---------|
| 1             | 2.15           | Fe    | NOG          | HIF-1α 786-826                 | 795-806                      | 812-823                     | 21.3                  | -                           | 1H2K    |
| 2             | 2.25           | Fe    | 2OG          | HIF-1α 786-826                 | 795-806                      | 813-822                     | 21.7                  | 0.149                       | 1H2L    |
| 3             | 2.50           | Zn    | NOG          | HIF-1α 775-826                 | 795-806                      | 813-822                     | 22.5                  | 0.136                       | 1H2M    |
| 4             | 2.84           | Fe    | 2OG          | HIF-2α 850-862                 | -                            | -                           | 25.7                  | 0.226                       | 1H2N    |

<sup>\*</sup> Crystalline FIH:CAD complexes were also obtained with Fe<sup>(II)</sup>, HIF-1α 775-786 and 2OG or NOG.

Methods employed in structural workProtein expression, purification and crystallisation

FIH, CAD<sub>775-826</sub> and CAD<sub>786-826</sub> were prepared as described (Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002). Selenomethionine (SeMet) substituted  
5 FIH was produced using a metabolic inhibition protocol and LeMaster media supplemented with 50 mg/l L-selenomethionine. SeMet incorporation was >95 % by ESI-MS. Aerobic crystallisation of SeMet FIH (at 11 mg ml<sup>-1</sup>) was accomplished by hanging-drop vapour diffusion at 17 °C. The mother liquor consisted of 1.2 M ammonium sulphate, 4 % PEG 400 and 0.1 M Hepes pH 7.5. Crystallisation of  
10 FIH:Fe:CAD fragment complexes was accomplished under an anaerobic atmosphere of argon in a Belle Technology glove box (0.3-0.4 ppm O<sub>2</sub>) using the same mother liquor and a solution containing FIH (at 11 mg ml<sup>-1</sup>), Fe<sup>2+</sup> (1 mM), 2OG/NOG (2 mM) and CAD fragment (1 mM). Crystallisation of FIH:Zn:CAD fragment was accomplished aerobically under similar conditions. Peptides were either synthesised  
15 by solid phase peptide synthesis or purchased from Biopeptide Co. (San Diego, USA).

Crystallographic data collection and structure refinement

Crystals were cryocooled by plunging into liquid nitrogen and X-ray data  
20 were collected at 100 K using a nitrogen stream. Cryoprotection was accomplished by sequential transfer into a solution containing 1.2 M ammonium sulphate, 3 % PEG 400, 0.1 M Hepes pH 7.5 and 10 % followed by 24 % glycerol. A three-wavelength multiple anomalous dispersion (MAD) dataset was collected to 2.9 Å resolution on beamline 14.2 of the Synchrotron Radiation Source, Daresbury, U.K.  
25 Data from crystals of FIH:CAD complexes were collected on beamlines 14.2, 9.6 or 9.5 using ADSC Quantum 4 (14.2 and 9.6) or MarCCD detectors (9.5). All data was processed with the program MOSFLM and the CCP4 suite[Collaborative Computational Project Number 4 *Acta Crystallogr.* **D50**, 760-763 (1994)]. The crystals belonged to space group *P*4<sub>1</sub>2<sub>1</sub>2. Six selenium positions were located and  
30 phases calculated using the program SOLVE (Terwilliger et al. **D55**, 849-861, 1999). Density modification, which increased the figure of merit from 0.56 to 0.66, was performed using RESOLVE (Terwilliger *Acta Crystallogr.* **D56**, 965-972 2000).

An initial model was built using the program O (Jones et al, *Acta Crystallogr.* A47, 110-119, 1991).and refined against the SeMet data (remote wavelength) using the program CNS (Brunger *Acta Crystallogr.* D54, 905-921, 1998). . One cycle of simulated annealing followed by grouped *B*-factor refinement brought the  $R_{\text{free}}$  to 36.2 %. Following further rebuilding and refinement, which brought the  $R_{\text{free}}$  to 32.3 %, the model was transferred to the 2.15 Å dataset. Rebuilding and refinement using REFMAC5 including addition of Fe, substrate and solvent molecules, and refinement of TLS parameters brought the conventional *R*-factor to 17.8 % and the  $R_{\text{free}}$  to 21.3 %. The following residues are missing in the current model: 1-15 and 304-306 of FIH, 786-794, 807-811 and 824-826 of the CAD fragment. According to PROCHECK there are no Ramachandran outliers and 90.7 % of residues have most favourable backbone conformations. For the CAD peptide, 77.8% of residues are in the most favourable region with the remaining 22.2 % in additionally allowed regions.

Other structures were solved by molecular replacement using the coordinates from the 2.15 Å data and refinement using REFMAC5. In all structures electron density for the Fe and 2OG/NOG was visible throughout refinement. Significant positive difference electron density was observed between the iron and the CAD Asn803  $\beta$ -carbon. Since *B*-factor differences between FIH and CAD imply that the CAD is not at 100 % occupancy, this may represent an alternative binding-mode for the 1-carboxylate 2OG in the absence of substrate although it could also be due to a ligating water molecule, again in the absence of substrate.

#### Overview of FIH structure

The core of FIH comprises a double-stranded beta-helix (DSBH or jellyroll) motif formed from eight  $\beta$ -strands,  $\beta 8$ - $\beta 11$  and  $\beta 14$ - $\beta 17$ . Residues 220-259 form an insert between strands 4 and 5 of the DSBH. The bottom face of the DSBH is flanked by an additional four  $\beta$ -strands from the N-terminal region to form an eight-membered antiparallel  $\beta$ -sheet. The N-terminal strand  $\beta 1$  bisects the face of the DSBH opposite to the active site. The  $\beta 1$  strand has a 360° twist located at a PXXP sequence, in between its interactions with  $\beta 14$  and  $\beta 2$ . A similarly positioned  $\beta$ -

strand is found in most 2OG oxygenases, though not always from the same region of the protein. The sheet-helix-sheet motif formed by  $\beta 1$ ,  $\alpha 1$  and  $\beta 2$  is conserved in all enzymes of this class except proline 3-hydroxylase and a similar fold in this region is found in the related  $\text{Cu}^{(\text{II})}$  utilising quercetin 2,3-dioxygenase (QD) (Fusetti et al, 5 STRUCTURE 10 (2): 259-268 2002). The topology of FIH unequivocally defines it as an iron-binding member of the cupin structural family which already includes QD and  $\text{Mn}^{(\text{II})}$  utilising Type II phosphomannose isomerase (Clissold, P. M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* 26, 79).

#### 10 Related enzymes to FIH

FIH has significant sequence similarity with the JmjC homology region of the jumonji transcription factors (Clissold, P. M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* 26, 79; Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002). These proteins are members of the cupin structural superfamily and have been 15 implicated in cell growth and heart development. The 2OG oxygenase iron binding residues had been identified in some JmjC domains but not assigned as an iron binding motif. Sequence searches in the light of the FIH structure reveal many JmjC proteins with conserved residues that include both this motif and others, including FIH residues Lys214 and Thr196 that are unusually involved in binding the 5- 20 carboxylate of 2OG. The structure thus reveals that FIH is a one of a large family of iron and 2OG dependent oxygenases involved in the regulation of transcription. Since some of the assigned JmjC domains other than FIH are associated with diseases and particular phenotypes their (e.g.) inhibition may be of therapeutic value. (See e.g. Hu et al, ONCOGENE 20 (47): 6946-6954 OCT 18 2001 and Clissold, P. 25 M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* 26, 79 and references therein).

Table 2. Partial sequence alignment of FIH with a selection of JmjC domain containing proteins. FIH secondary structure is indicated above the alignment. Selected 2OG binding residues found in FIH are indicated by dark triangles under the alignment and the two iron binding residues by light triangles. SWALL accession 30 numbers are indicated on the left of the alignment.



|     | $\alpha 7$ | $\beta 8$ | $\beta 9$        | $\beta 10$      | $\beta 11$       |                 |                 |                 |                |
|-----|------------|-----------|------------------|-----------------|------------------|-----------------|-----------------|-----------------|----------------|
| FIH | Q969Q7     | HS        | FNWNWINKQQ       | -----GKRGWQ     | -----LTSNLLLI    | MEGNVTFAHYDEQ   | -----QNFQAQIKGY | -----KRCILFPPD  |                |
| Dm  | Q9VU77     | Dm        | -----ELAADLR     | -----VSDLDEAQ   | (4) -PPDAVNFWI   | DERAVTSMHKDPY   | -----ENVYCVISGH | -----KDFVLLPPH  |                |
| Dm  | Q9W0M3     | Dm        | -----ALKEDIS     | -----IPDYCTI    | (5) PGAVDIKAWL   | PAGTVSEPMHYDEK  | -----HNLICQVFGS | -----KRILLAAPA  |                |
| HS  | Q9UPP1     | HS        | -----KIVRKLS     | -----WVENLWPEEC | (4) PNVQKCYCLMS  | VRDSYTDHIDFGGT  | -----SVWYHVLKGE | -----KIFYLIRPT  |                |
| Ce  | Q9BI67     | Ce        | -----RFVQEIS     | -----MVNRLWEDY  | (20) PKVEQFCIA   | MAGSYTDFHVDFFGS | -----SVYYHILKGE | -----KIFYTAAPT  |                |
| Ce  | Q20367     | Ce        | -----RFVQDIS     | -----MAKRLWSDV  | (11) PKIEQICAA   | AMANSYTDHVDFFGT | -----SVYFHVFKGE | (4) KIFYTAAPT   |                |
| Dm  | Q9VHH9     | Dm        | -----EIVRQID     | -----WVDVWPKQ   | (16) PKVQKCYCLMS | VKNCTDHFHIDFGGT | -----SVWYHILRGS | (1) KVFLLIRPT   |                |
| SSC | P40034     | SSC       | -----QNDLVDKIW   | -----SFNGHLEKY  | (11) PKVTKYILMS  | VKDAYTDFHLDFACT | -----SVYYNVVISQ | -----KKELLEPPPT |                |
| Rn  | Q9R153     | Rn        | -----KTDVFEQVM   | -----WSDFGEP    | -----RNGQE       | -----STLWI      | SLGAHTPCHLDSYG  | -----CNLVFQVQGR | -----KRWHLEPPE |
| Ce  | Q9GYI4     | Ce        | -----FEDDLFHYAD  | -----DKKRPPH    | -----RWFTVM      | PARSGTATHIDPLG  | TSAMNSLLQGH     | -----KRWVLIPTI  |                |
| Dm  | Q9V6L0     | Dm        | -----TILDYVVKDYN | IQIDVNT         | -----AYLYF       | EMKTFEAWHTEDMD  | LYSINYLHFGAP    | -----KTYVYVVRPE |                |
| HS  | Q94877     | HS        | -----TVLDVVEECG  | ISIECVNT        | -----PYLYF       | EMKTFEAWHTEDMD  | LYSINYLHFGEP    | -----RSWYAIAPPE |                |
| Ce  | Q9U297     | Ce        | -----TILEDNTYE   | -----IKFVNT     | -----VYLYF       | MYKTFEAWHTEDMD  | LYSINYLHFGAP    | -----KYWFAISSE  |                |
| Dm  | Q9V333     | Dm        | -----TILNLVNTDYN | IIIDVNT         | -----AXLYF       | EMKTSFAWHTEDMD  | LYSINYLHFGAP    | -----KTYWAIPTA  |                |
| HS  | Q75164     | HS        | -----TILDLVEKESG | TIEGVNT         | -----PYLYF       | EMKTSFAWHTEDMD  | LYSINYLHFGEP    | -----KSWYSVPPE  |                |
| Dm  | Q9VJ97     | Dm        | -----FASDWLNEQL  | -----IQCKDDY    | -----RFVYM       | PKNSWTSTSYHADV  | FGESWSTNTIVGL   | -----KKWLJMPPG  |                |
| Sp  | Q13977     | Sp        | -----FADDWLNAVY  | -----IDCESDDF   | -----RFAYL       | SHLTTTGLHTDVY   | ASHSESVNLCGV    | -----KCWLFIIDPK |                |

FIH = Factor Inhibiting HIF  
 PASS1 = Protein associating with  
 small stress protein

Hs = Homo sapiens  
 Dm = Drosophila melanogaster  
 Ce = Caenorhabditis elegans  
 Sc = Saccharomyces cerevisiae  
 Rn = Rattus norvegicus  
 Sp = Schizosaccharomyces pombe

TABLE 2

TABLE 3 - Coordinates for structures 1 to 4

Structure 1

Below are the coordinates for structure 1 (the 2.15 Å structure of FIH:Fe(II):NOG:CAD):

```

HEADER      TRANSCRIPTION ACTIVATOR/INHIBITOR      12-AUG-02   1H2K
TITLE       FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE       2 FRAGMENT PEPTIDE
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND      3 CHAIN: A;
COMPND      4 ENGINEERED: YES;
COMPND      5 MOL_ID: 2;
COMPND      6 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND      7 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
COMPND      8 MEMBER OF PAS PROTEIN 1;
COMPND      9 CHAIN: S;
COMPND     10 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND     11 RESIDUES 786-826
SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE      3 ORGANISM_COMMON: HUMAN;
SOURCE      4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE      5 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE      6 EXPRESSION_SYSTEM_PLASMID: PET28A(+);
SOURCE      7 MOL_ID: 2;
SOURCE      8 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE      9 ORGANISM_COMMON: HUMAN;
SOURCE     10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE     11 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE     12 EXPRESSION_SYSTEM_PLASMID: PGEX-GP-1
KEYWDS      FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
KEYWDS      2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, PHOSPHORYLATION
EXPDTA      X-RAY DIFFRACTION
AUTHOR      J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,I.SCHLEMMINGER,
AUTHOR      2 J.F.SEIBEL,C.J.SCHOFIELD
REVDAT      1   03-SEP-02 1H2K   0
JRNL        AUTH   J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,
JRNL        AUTH 2 I.SCHLEMMINGER,J.F.SEIBEL,C.J.SCHOFIELD
JRNL        TITL   FIH:HIF-FRAGMENT COMPLEXES
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK      2
REMARK      2 RESOLUTION. 2.15 ANGSTROMS.
REMARK      3
REMARK      3 REFINEMENT.
REMARK      3   PROGRAM      : REFMAC 5.0
REMARK      3   AUTHORS      : MURSHUDOV,VAGIN,DODSON
REMARK      3
REMARK      3   REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK      3
REMARK      3 DATA USED IN REFINEMENT.
REMARK      3   RESOLUTION RANGE HIGH (ANGSTROMS) :   2.15
REMARK      3   RESOLUTION RANGE LOW  (ANGSTROMS) :  18.50
REMARK      3   DATA CUTOFF          (SIGMA(F)) : NONE
REMARK      3   COMPLETENESS FOR RANGE          (%) :  99.28
REMARK      3   NUMBER OF REFLECTIONS              :  28171
REMARK      3

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```

REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE (WORKING + TEST SET) : 0.18026
REMARK 3 R VALUE (WORKING SET) : 0.17761
REMARK 3 FREE R VALUE : 0.21305
REMARK 3 FREE R VALUE TEST SET SIZE (%) : 7.7
REMARK 3 FREE R VALUE TEST SET COUNT : 2340
REMARK 3
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK 3 TOTAL NUMBER OF BINS USED : 20
REMARK 3 BIN RESOLUTION RANGE HIGH : 2.150
REMARK 3 BIN RESOLUTION RANGE LOW : 2.205
REMARK 3 REFLECTION IN BIN (WORKING SET) : 1906
REMARK 3 BIN R VALUE (WORKING SET) : 0.222
REMARK 3 BIN FREE R VALUE SET COUNT : 152
REMARK 3 BIN FREE R VALUE : 0.257
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS : 2875
REMARK 3 NUCLEIC ACID ATOMS : 0
REMARK 3 HETEROGEN ATOMS : 21
REMARK 3 SOLVENT ATOMS : 194
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2) : NULL
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 25.725
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : -0.27
REMARK 3 B22 (A**2) : -0.27
REMARK 3 B33 (A**2) : 0.55
REMARK 3 B12 (A**2) : 0.00
REMARK 3 B13 (A**2) : 0.00
REMARK 3 B23 (A**2) : 0.00
REMARK 3
REMARK 3 ESTIMATED OVERALL COORDINATE ERROR.
REMARK 3 ESU BASED ON R VALUE (A) : 0.174
REMARK 3 ESU BASED ON FREE R VALUE (A) : 0.156
REMARK 3 ESU BASED ON MAXIMUM LIKELIHOOD (A) : 0.147
REMARK 3 ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2) : 5.588
REMARK 3
REMARK 3 CORRELATION COEFFICIENTS.
REMARK 3 CORRELATION COEFFICIENT FO-FC : 0.961
REMARK 3 CORRELATION COEFFICIENT FO-FC FREE : 0.947
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES COUNT RMS WEIGHT
REMARK 3 BOND LENGTHS REFINED (A) : 2973 ; 0.012 ; 0.021
REMARK 3 BOND LENGTHS OTHERS (A) : 2561 ; 0.001 ; 0.020
REMARK 3 BOND ANGLES REFINED (DEGREES) : 4044 ; 1.374 ; 1.949
REMARK 3 BOND ANGLES OTHERS (DEGREES) : 5979 ; 0.722 ; 3.000
REMARK 3 TORSION ANGLES, PERIOD 1 (DEGREES) : 352 ; 4.018 ; 3.000
REMARK 3 TORSION ANGLES, PERIOD 3 (DEGREES) : 515 ; 17.698 ; 15.000
REMARK 3 CHIRAL-CENTER RESTRAINTS (A**3) : 416 ; 0.086 ; 0.200
REMARK 3 GENERAL PLANES REFINED (A) : 3333 ; 0.005 ; 0.020
REMARK 3 GENERAL PLANES OTHERS (A) : 604 ; 0.002 ; 0.020
REMARK 3 NON-BONDED CONTACTS REFINED (A) : 714 ; 0.218 ; 0.300
REMARK 3 NON-BONDED CONTACTS OTHERS (A) : 2499 ; 0.204 ; 0.300
REMARK 3 H-BOND (X...Y) REFINED (A) : 259 ; 0.152 ; 0.500
REMARK 3 H-BOND (X...Y) OTHERS (A) : 4 ; 0.087 ; 0.500
REMARK 3 SYMMETRY VDW REFINED (A) : 18 ; 0.245 ; 0.300
REMARK 3 SYMMETRY VDW OTHERS (A) : 72 ; 0.248 ; 0.300

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REMARK 3 SYMMETRY H-BOND REFINED (A): 13 ; 0.255 ; 0.500  
 REMARK 3 SYMMETRY H-BOND OTHERS (A): 1 ; 0.052 ; 0.500  
 REMARK 3  
 REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS COUNT RMS WEIGHT  
 REMARK 3 MAIN-CHAIN BOND REFINED (A\*\*2): 1777 ; 0.618 ; 1.500  
 REMARK 3 MAIN-CHAIN ANGLE REFINED (A\*\*2): 2862 ; 1.177 ; 2.000  
 REMARK 3 SIDE-CHAIN BOND REFINED (A\*\*2): 1196 ; 1.812 ; 3.000  
 REMARK 3 SIDE-CHAIN ANGLE REFINED (A\*\*2): 1182 ; 3.002 ; 4.500  
 REMARK 3  
 REMARK 3 NCS RESTRAINTS STATISTICS  
 REMARK 3 NUMBER OF NCS GROUPS : NULL  
 REMARK 3  
 REMARK 3 TLS DETAILS  
 REMARK 3 NUMBER OF TLS GROUPS : 1  
 REMARK 3  
 REMARK 3 TLS GROUP : 1  
 REMARK 3 NUMBER OF COMPONENTS GROUP : 2  
 REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI  
 REMARK 3 RESIDUE RANGE : A 15 A 451  
 REMARK 3 RESIDUE RANGE : S 795 S 823  
 REMARK 3 ORIGIN FOR THE GROUP (A): 21.6620 27.4620 28.2370  
 REMARK 3 T TENSOR  
 REMARK 3 T11: 0.1474 T22: 0.0149  
 REMARK 3 T33: 0.0919 T12: -0.0099  
 REMARK 3 T13: -0.0455 T23: 0.0363  
 REMARK 3 L TENSOR  
 REMARK 3 L11: 1.0098 L22: 2.2577  
 REMARK 3 L33: 1.2037 L12: 0.6963  
 REMARK 3 L13: 0.4840 L23: 1.0420  
 REMARK 3 S TENSOR  
 REMARK 3 S11: 0.0288 S12: -0.1525 S13: -0.0400  
 REMARK 3 S21: 0.1459 S22: 0.0002 S23: 0.1021  
 REMARK 3 S31: 0.1876 S32: -0.0468 S33: -0.0290  
 REMARK 3  
 REMARK 3 BULK SOLVENT MODELLING.  
 REMARK 3 METHOD USED : BABINET MODEL WITH MASK  
 REMARK 3 PARAMETERS FOR MASK CALCULATION  
 REMARK 3 VDW PROBE RADIUS : 1.40  
 REMARK 3 ION PROBE RADIUS : 0.80  
 REMARK 3 SHRINKAGE RADIUS : 0.80  
 REMARK 3  
 REMARK 3 OTHER REFINEMENT REMARKS: HYDROGENS HAVE BEEN ADDED IN THE  
 REMARK 3 RIDING POSITIONS  
 REMARK 4  
 REMARK 4 1H2K COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998  
 REMARK 100  
 REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.  
 REMARK 100 THE EBI ID CODE IS EBI-11170.  
 REMARK 200  
 REMARK 200 EXPERIMENTAL DETAILS  
 REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION  
 REMARK 200 DATE OF DATA COLLECTION : 15-MAY-2002  
 REMARK 200 TEMPERATURE (KELVIN) : 100  
 REMARK 200 PH : 7.5  
 REMARK 200 NUMBER OF CRYSTALS USED : 1  
 REMARK 200  
 REMARK 200 SYNCHROTRON (Y/N) : Y  
 REMARK 200 RADIATION SOURCE : SRS BEAMLINE PX9.6  
 REMARK 200 BEAMLINE : PX9.6  
 REMARK 200 X-RAY GENERATOR MODEL : NULL  
 REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M



REMARK 200 WAVELENGTH OR RANGE (A) : 0.87  
REMARK 200 MONOCHROMATOR : NULL  
REMARK 200 OPTICS : NULL  
REMARK 200  
REMARK 200 DETECTOR TYPE : CCD  
REMARK 200 DETECTOR MANUFACTURER : ADSC  
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : MOSFLM  
REMARK 200 DATA SCALING SOFTWARE : SCALE  
REMARK 200  
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 30574  
REMARK 200 RESOLUTION RANGE HIGH (A) : 2.15  
REMARK 200 RESOLUTION RANGE LOW (A) : 18.17  
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NONE  
REMARK 200  
REMARK 200 OVERALL.  
REMARK 200 COMPLETENESS FOR RANGE (%) : 99.2  
REMARK 200 DATA REDUNDANCY : 6.3  
REMARK 200 R MERGE (I) : 0.052  
REMARK 200 R SYM (I) : NULL  
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 9.9  
REMARK 200  
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.  
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.15  
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A) : 2.27  
REMARK 200 COMPLETENESS FOR SHELL (%) : 96.0  
REMARK 200 DATA REDUNDANCY IN SHELL : 3.4  
REMARK 200 R MERGE FOR SHELL (I) : 0.331  
REMARK 200 R SYM FOR SHELL (I) : NULL  
REMARK 200 <I/SIGMA(I)> FOR SHELL : 1.5  
REMARK 200  
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH  
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MAD  
REMARK 200 SOFTWARE USED: SOLVE  
REMARK 200 STARTING MODEL: NULL  
REMARK 200  
REMARK 200 REMARK: NULL  
REMARK 280  
REMARK 280 CRYSTAL  
REMARK 280 SOLVENT CONTENT, VS (%): 63  
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS\*\*3/DA): 3.4  
REMARK 280  
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE, 4% PEG400,  
REMARK 280 0.1M HEPES PH7.5, ARGON ATMOSPHERE, 11MG/ML PROTEIN WITH  
REMARK 280 1MM FE(II), 2.5MM NOG AND 2.5MM PEPTIDE  
REMARK 290  
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY  
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2  
REMARK 290  
REMARK 290 SYMOP SYMMETRY  
REMARK 290 NNNMMM OPERATOR  
REMARK 290 1555 X, Y, Z  
REMARK 290 2555 -X, -Y, 1/2+Z  
REMARK 290 3555 1/2-Y, 1/2+X, 1/4+Z  
REMARK 290 4555 1/2+Y, 1/2-X, 3/4+Z  
REMARK 290 5555 1/2-X, 1/2+Y, 1/4-Z  
REMARK 290 6555 1/2+X, 1/2-Y, 3/4-Z  
REMARK 290 7555 Y, X, -Z  
REMARK 290 8555 -Y, -X, 1/2-Z  
REMARK 290  
REMARK 290 WHERE NNN -> OPERATOR NUMBER  
REMARK 290 MMM -> TRANSLATION VECTOR

REMARK 290

REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS

REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM

REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY

REMARK 290 RELATED MOLECULES.

|            |        |   |           |           |           |           |
|------------|--------|---|-----------|-----------|-----------|-----------|
| REMARK 290 | SMTRY1 | 1 | 1.000000  | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 1 | 0.000000  | 1.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 1 | 0.000000  | 0.000000  | 1.000000  | 0.000000  |
| REMARK 290 | SMTRY1 | 2 | -1.000000 | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 2 | 0.000000  | -1.000000 | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 2 | 0.000000  | 0.000000  | 1.000000  | 73.32800  |
| REMARK 290 | SMTRY1 | 3 | 0.000000  | -1.000000 | 0.000000  | 43.08050  |
| REMARK 290 | SMTRY2 | 3 | 1.000000  | 0.000000  | 0.000000  | 43.08050  |
| REMARK 290 | SMTRY3 | 3 | 0.000000  | 0.000000  | 1.000000  | 36.66400  |
| REMARK 290 | SMTRY1 | 4 | 0.000000  | 1.000000  | 0.000000  | 43.08050  |
| REMARK 290 | SMTRY2 | 4 | -1.000000 | 0.000000  | 0.000000  | 43.08050  |
| REMARK 290 | SMTRY3 | 4 | 0.000000  | 0.000000  | 1.000000  | 109.99200 |
| REMARK 290 | SMTRY1 | 5 | -1.000000 | 0.000000  | 0.000000  | 43.08050  |
| REMARK 290 | SMTRY2 | 5 | 0.000000  | 1.000000  | 0.000000  | 43.08050  |
| REMARK 290 | SMTRY3 | 5 | 0.000000  | 0.000000  | -1.000000 | 36.66400  |
| REMARK 290 | SMTRY1 | 6 | 1.000000  | 0.000000  | 0.000000  | 43.08050  |
| REMARK 290 | SMTRY2 | 6 | 0.000000  | -1.000000 | 0.000000  | 43.08050  |
| REMARK 290 | SMTRY3 | 6 | 0.000000  | 0.000000  | -1.000000 | 109.99200 |
| REMARK 290 | SMTRY1 | 7 | 0.000000  | 1.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 7 | 1.000000  | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 7 | 0.000000  | 0.000000  | -1.000000 | 0.000000  |
| REMARK 290 | SMTRY1 | 8 | 0.000000  | -1.000000 | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 8 | -1.000000 | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 8 | 0.000000  | 0.000000  | -1.000000 | 73.32800  |

REMARK 290

REMARK 290 REMARK: NULL

REMARK 300

REMARK 300 BIOMOLECULE: 1

REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT

REMARK 300 WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR

REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).

REMARK 300

REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC

REMARK 300

REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.

REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S

REMARK 300 PRODUCES A TETRAMER.

REMARK 300

REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE

REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT

REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE

REMARK 300 HOMODIMER OF CHAIN A

REMARK 300

REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS

REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH

REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER

REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR

REMARK 300 THE CHAIN IN THE COMPLEX IS 2203.4 ANGSTROM\*\*2

REMARK 350

REMARK 350 GENERATING THE BIOMOLECULE

REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN

REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE

REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS

REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND

REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.

REMARK 350

REMARK 350 BIOMOLECULE: 1  
 REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S  

|            |        |   |           |           |           |          |
|------------|--------|---|-----------|-----------|-----------|----------|
| REMARK 350 | BIOMT1 | 1 | 1.000000  | 0.000000  | 0.000000  | 0.000000 |
| REMARK 350 | BIOMT2 | 1 | 0.000000  | 1.000000  | 0.000000  | 0.000000 |
| REMARK 350 | BIOMT3 | 1 | 0.000000  | 0.000000  | 1.000000  | 0.000000 |
| REMARK 350 | BIOMT1 | 2 | 0.000000  | -1.000000 | 0.000000  | 86.16100 |
| REMARK 350 | BIOMT2 | 2 | -1.000000 | 0.000000  | 0.000000  | 86.16100 |
| REMARK 350 | BIOMT3 | 2 | 0.000000  | 0.000000  | -1.000000 | 73.32800 |

REMARK 465

REMARK 465 MISSING RESIDUES

REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE  
 REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN  
 REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)

REMARK 465

REMARK 465 M RES C SSSEQI

|            |     |   |     |
|------------|-----|---|-----|
| REMARK 465 | MET | A | 1   |
| REMARK 465 | ALA | A | 2   |
| REMARK 465 | ALA | A | 3   |
| REMARK 465 | THR | A | 4   |
| REMARK 465 | ALA | A | 5   |
| REMARK 465 | ALA | A | 6   |
| REMARK 465 | GLU | A | 7   |
| REMARK 465 | ALA | A | 8   |
| REMARK 465 | VAL | A | 9   |
| REMARK 465 | ALA | A | 10  |
| REMARK 465 | SER | A | 11  |
| REMARK 465 | GLY | A | 12  |
| REMARK 465 | SER | A | 13  |
| REMARK 465 | GLY | A | 14  |
| REMARK 465 | LYS | A | 304 |
| REMARK 465 | ARG | A | 305 |
| REMARK 465 | ILE | A | 306 |
| REMARK 465 | SER | S | 786 |
| REMARK 465 | MET | S | 787 |
| REMARK 465 | ASP | S | 788 |
| REMARK 465 | GLU | S | 789 |
| REMARK 465 | SER | S | 790 |
| REMARK 465 | GLY | S | 791 |
| REMARK 465 | LEU | S | 792 |
| REMARK 465 | PRO | S | 793 |
| REMARK 465 | GLN | S | 794 |
| REMARK 465 | GLN | S | 807 |
| REMARK 465 | GLY | S | 808 |
| REMARK 465 | SER | S | 809 |
| REMARK 465 | ARG | S | 810 |
| REMARK 465 | ASN | S | 811 |
| REMARK 465 | GLN | S | 824 |
| REMARK 465 | VAL | S | 825 |
| REMARK 465 | ASN | S | 826 |

REMARK 470

REMARK 470 MISSING ATOM

REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;  
 REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;  
 REMARK 470 I=INSERTION CODE):

REMARK 470 M RES CSSEQI ATOMS

|            |     |   |     |    |     |     |            |
|------------|-----|---|-----|----|-----|-----|------------|
| REMARK 470 | GLU | A | 15  | CG | CD  | OE1 | OE2        |
| REMARK 470 | GLU | A | 29  | CG | CD  | OE1 | OE2        |
| REMARK 470 | ASN | A | 87  | CG | OD1 | ND2 |            |
| REMARK 470 | LYS | A | 106 | CD | CE  | NZ  |            |
| REMARK 470 | LYS | A | 115 | CG | CD  | CE  | NZ         |
| REMARK 470 | ARG | A | 117 | CG | CD  | NE  | CZ NH1 NH2 |

REMARK 470 GLN A 133 CG CD OE1 NE2  
 REMARK 470 GLN A 136 CG CD OE1 NE2  
 REMARK 470 GLN A 137 CG CD OE1 NE2  
 REMARK 470 ARG A 156 CG CD NE CZ NH1 NH2  
 REMARK 470 LYS A 157 CD CE NZ  
 REMARK 470 LYS A 311 CG CD CE NZ  
 REMARK 500  
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY  
 REMARK 500 SUBTOPIC: COVALENT BOND ANGLES  
 REMARK 500  
 REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES  
 REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE  
 REMARK 500 THAN 6\*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN  
 REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).  
 REMARK 500  
 REMARK 500 STANDARD TABLE:  
 REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)  
 REMARK 500  
 REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991  
 REMARK 500  
 REMARK 500 M RES CSSEQI ATM1 ATM2 ATM3  
 REMARK 500 ASN A 84 N - CA - C ANGL. DEV. = 9.3 DEGREES  
 REMARK 500  
 REMARK 500 REMARK: NULL  
 REMARK 500  
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY  
 REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS  
 REMARK 500  
 REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES  
 REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE  
 REMARK 500 THAN 6\*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL  
 REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE  
 REMARK 500 NUMBER; I=INSERTION CODE).  
 REMARK 500  
 REMARK 500 STANDARD TABLE:  
 REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,1X,2(A4,A1,3X),12X,F5.3)  
 REMARK 500  
 REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991  
 REMARK 500  
 REMARK 500 M RES CSSEQI ATM1 RES CSSEQI ATM2 DEVIATION  
 REMARK 500 MET A 343 SD MET A 343 CE -0.249  
 REMARK 500  
 REMARK 500 REMARK: NULL  
 REMARK 500  
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY  
 REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT  
 REMARK 500  
 REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.  
 REMARK 500  

| ATM1 | RES | C | SSEQI | ATM2 | RES | C | SSEQI | DISTANCE |
|------|-----|---|-------|------|-----|---|-------|----------|
| O    | GLN | A | 209   | O    | HOH | Z | 108   | 2.20     |

 REMARK 500  
 REMARK 525  
 REMARK 525 SOLVENT  
 REMARK 525  
 REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO  
 REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY  
 REMARK 525 ASSOCIATED WITH:  
 REMARK 525 PROTEIN CHAIN SOLVENT CHAIN  
 REMARK 525 A Z  
 REMARK 525 S H



REMARK 525

REMARK 525 THE FOLLOWING SOLVENT MOLECULES LIE FARTHER THAN EXPECTED  
 REMARK 525 FROM THE PROTEIN OR NUCLEIC ACID MOLECULE AND MAY BE  
 REMARK 525 ASSOCIATED WITH A SYMMETRY RELATED MOLECULE (M=MODEL  
 REMARK 525 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE  
 REMARK 525 NUMBER; I=INSERTION CODE):

REMARK 525

REMARK 525 THESE MOLECULES CAN BE PLACED WITHIN 5.00 ANGSTROM OF THE  
 REMARK 525 OBSERVED OLIGOMER BY APPLYING THE SYMMETRY TRANSFORMATION  
 REMARK 525 INDICATED.

REMARK 525

| M | RES | CSSEQI | ORIGINAL COORDINATES |        |        | SYMMETRY TRANS. |     | DIST. |
|---|-----|--------|----------------------|--------|--------|-----------------|-----|-------|
|   |     |        | X                    | Y      | Z      |                 |     |       |
| 1 | HOH | W 531  | 12.359               | 41.757 | 15.368 | 005             | 545 | 2.38  |
| 1 | HOH | W 609  | 10.971               | 45.216 | 18.991 | 005             | 545 | 3.25  |
| 1 | HOH | W 576  | 42.075               | 52.163 | 47.994 | 008             | 665 | 2.28  |
| 1 | HOH | W 687  | 28.879               | 5.577  | 12.106 | 005             | 555 | 2.82  |
| 1 | HOH | W 674  | 24.396               | 12.792 | 8.360  | 005             | 555 | 3.20  |
| 1 | HOH | W 543  | 27.797               | 7.178  | 14.664 | 005             | 555 | 2.83  |
| 1 | HOH | W 607  | 26.874               | 53.406 | 28.524 | 008             | 665 | 2.97  |

REMARK 600

REMARK 600 HETEROGEN

REMARK 600

REMARK 600 FOR METAL ATOM FE FE2 A1350 THE COORDINATION ANGLES ARE:

REMARK 600 1 HIS 199A NE2

REMARK 600 2 ASP 201A OD2 104.0

REMARK 600 3 HIS 279A NE2 85.8 88.0

REMARK 600 4 OGA 1351A O2 163.5 92.4 96.8

REMARK 600 5 OGA 1351A O2' 86.4 168.8 97.0 77.1

REMARK 600 1 2 3 4

REMARK 700

REMARK 700 SHEET

REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN  
 REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,  
 REMARK 700 TWO SHEETS ARE DEFINED.

REMARK 800

REMARK 800 SITE

REMARK 800 SITE\_IDENTIFIER: FE1

REMARK 800 SITE\_DESCRIPTION: FE BINDING SITE FOR CHAIN A

REMARK 800

REMARK 800 SITE\_IDENTIFIER: OGA

REMARK 800 SITE\_DESCRIPTION: OGA BINDING SITE FOR CHAIN A

REMARK 800

REMARK 800 SITE\_IDENTIFIER: SO1

REMARK 800 SITE\_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A

REMARK 800

REMARK 800 SITE\_IDENTIFIER: SO2

REMARK 800 SITE\_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A

REMARK 900

REMARK 900 RELATED ENTRIES

REMARK 900 RELATED ID: 1D7G RELATED DB: PDB

REMARK 900 A MODEL FOR THE COMPLEX BETWEEN THE

REMARK 900 HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS

REMARK 900 CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE

REMARK 900 RELATED ID: 1H2L RELATED DB: PDB

REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX

REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE

REMARK 900 RELATED ID: 1H2M RELATED DB: PDB

REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX

REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE

REMARK 900 RELATED ID: 1H2N RELATED DB: PDB

REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX  
 REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE  
 REMARK 900 RELATED ID: 1L8C RELATED DB: PDB  
 REMARK 900 STRUCTURAL BASIS FOR HIF-1ALPHA/CBP  
 REMARK 900 RECOGNITION IN THECELLULAR HYPOXIC RESPONSE  
 REMARK 900 RELATED ID: 1LM8 RELATED DB: PDB  
 REMARK 900 STRUCTURE OF A HIF-1A-PVHL-ELONGINB-  
 REMARK 900 ELONGINC COMPLEX  
 REMARK 900 RELATED ID: 1LQB RELATED DB: PDB  
 REMARK 900 CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1  
 REMARK 900 ALPHA PEPTIDEBOUND TO THE PVHL/ELONGIN-C/  
 REMARK 900 ELONGIN-B COMPLEX

|       |      |   |     |     |     |        |            |     |     |
|-------|------|---|-----|-----|-----|--------|------------|-----|-----|
| DBREF | 1H2K | A | 1   | 349 | SWS | Q969Q7 | Q969Q7     | 1   | 349 |
| DBREF | 1H2K | S | 786 | 826 | SWS | Q16665 | HIFA_HUMAN | 786 | 826 |

|        |    |   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|--------|----|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SEQRES | 1  | A | 349 | MET | ALA | ALA | THR | ALA | ALA | GLU | ALA | VAL | ALA | SER | GLY | SER |
| SEQRES | 2  | A | 349 | GLY | GLU | PRO | ARG | GLU | GLU | ALA | GLY | ALA | LEU | GLY | PRO | ALA |
| SEQRES | 3  | A | 349 | TRP | ASP | GLU | SER | GLN | LEU | ARG | SER | TYR | SER | PHE | PRO | THR |
| SEQRES | 4  | A | 349 | ARG | PRO | ILE | PRO | ARG | LEU | SER | GLN | SER | ASP | PRO | ARG | ALA |
| SEQRES | 5  | A | 349 | GLU | GLU | LEU | ILE | GLU | ASN | GLU | GLU | PRO | VAL | VAL | LEU | THR |
| SEQRES | 6  | A | 349 | ASP | THR | ASN | LEU | VAL | TYR | PRO | ALA | LEU | LYS | TRP | ASP | LEU |
| SEQRES | 7  | A | 349 | GLU | TYR | LEU | GLN | GLU | ASN | ILE | GLY | ASN | GLY | ASP | PHE | SER |
| SEQRES | 8  | A | 349 | VAL | TYR | SER | ALA | SER | THR | HIS | LYS | PHE | LEU | TYR | TYR | ASP |
| SEQRES | 9  | A | 349 | GLU | LYS | LYS | MET | ALA | ASN | PHE | GLN | ASN | PHE | LYS | PRO | ARG |
| SEQRES | 10 | A | 349 | SER | ASN | ARG | GLU | GLU | MET | LYS | PHE | HIS | GLU | PHE | VAL | GLU |
| SEQRES | 11 | A | 349 | LYS | LEU | GLN | ASP | ILE | GLN | GLN | ARG | GLY | GLY | GLU | GLU | ARG |
| SEQRES | 12 | A | 349 | LEU | TYR | LEU | GLN | GLN | THR | LEU | ASN | ASP | THR | VAL | GLY | ARG |
| SEQRES | 13 | A | 349 | LYS | ILE | VAL | MET | ASP | PHE | LEU | GLY | PHE | ASN | TRP | ASN | TRP |
| SEQRES | 14 | A | 349 | ILE | ASN | LYS | GLN | GLN | GLY | LYS | ARG | GLY | TRP | GLY | GLN | LEU |
| SEQRES | 15 | A | 349 | THR | SER | ASN | LEU | LEU | LEU | ILE | GLY | MET | GLU | GLY | ASN | VAL |
| SEQRES | 16 | A | 349 | THR | PRO | ALA | HIS | TYR | ASP | GLU | GLN | GLN | ASN | PHE | PHE | ALA |
| SEQRES | 17 | A | 349 | GLN | ILE | LYS | GLY | TYR | LYS | ARG | CYS | ILE | LEU | PHE | PRO | PRO |
| SEQRES | 18 | A | 349 | ASP | GLN | PHE | GLU | CYS | LEU | TYR | PRO | TYR | PRO | VAL | HIS | HIS |
| SEQRES | 19 | A | 349 | PRO | CYS | ASP | ARG | GLN | SER | GLN | VAL | ASP | PHE | ASP | ASN | PRO |
| SEQRES | 20 | A | 349 | ASP | TYR | GLU | ARG | PHE | PRO | ASN | PHE | GLN | ASN | VAL | VAL | GLY |
| SEQRES | 21 | A | 349 | TYR | GLU | THR | VAL | VAL | GLY | PRO | GLY | ASP | VAL | LEU | TYR | ILE |
| SEQRES | 22 | A | 349 | PRO | MET | TYR | TRP | TRP | HIS | HIS | ILE | GLU | SER | LEU | LEU | ASN |
| SEQRES | 23 | A | 349 | GLY | GLY | ILE | THR | ILE | THR | VAL | ASN | PHE | TRP | TYR | LYS | GLY |
| SEQRES | 24 | A | 349 | ALA | PRO | THR | PRO | LYS | ARG | ILE | GLU | TYR | PRO | LEU | LYS | ALA |
| SEQRES | 25 | A | 349 | HIS | GLN | LYS | VAL | ALA | ILE | MET | ARG | ASN | ILE | GLU | LYS | MET |
| SEQRES | 26 | A | 349 | LEU | GLY | GLU | ALA | LEU | GLY | ASN | PRO | GLN | GLU | VAL | GLY | PRO |
| SEQRES | 27 | A | 349 | LEU | LEU | ASN | THR | MET | ILE | LYS | GLY | ARG | TYR | ASN |     |     |
| SEQRES | 1  | S | 41  | SER | MET | ASP | GLU | SER | GLY | LEU | PRO | GLN | LEU | THR | SER | TYR |
| SEQRES | 2  | S | 41  | ASP | CYS | GLU | VAL | ASN | ALA | PRO | ILE | GLN | GLY | SER | ARG | ASN |
| SEQRES | 3  | S | 41  | LEU | LEU | GLN | GLY | GLU | GLU | LEU | LEU | ARG | ALA | LEU | ASP | GLN |
| SEQRES | 4  | S | 41  | VAL | ASN |     |     |     |     |     |     |     |     |     |     |     |

|     |     |       |    |
|-----|-----|-------|----|
| HET | FE2 | A1350 | 1  |
| HET | OGA | A1351 | 10 |
| HET | SO4 | A1352 | 5  |
| HET | SO4 | A1353 | 5  |

|        |     |                  |
|--------|-----|------------------|
| HETNAM | FE2 | FE (II) ION      |
| HETNAM | OGA | N-OXALYOLGLYCINE |
| HETNAM | SO4 | SULFATE ION      |

|        |   |     |             |
|--------|---|-----|-------------|
| FORMUL | 3 | FE2 | FE1 2+      |
| FORMUL | 4 | OGA | C4 H5 N1 O5 |
| FORMUL | 5 | SO4 | 2(O4 S1 2-) |
| FORMUL | 6 | HOH | *194(H2 O1) |

|       |   |   |     |   |     |     |   |     |   |
|-------|---|---|-----|---|-----|-----|---|-----|---|
| HELIX | 1 | 1 | ASP | A | 28  | LEU | A | 32  | 5 |
| HELIX | 2 | 2 | ASP | A | 49  | ASN | A | 58  | 1 |
| HELIX | 3 | 3 | VAL | A | 70  | TRP | A | 76  | 5 |
| HELIX | 4 | 4 | ASP | A | 77  | ILE | A | 85  | 1 |
| HELIX | 5 | 5 | ASP | A | 104 | GLN | A | 112 | 5 |

5  
10  
7  
9  
9



|      |    |     |     |   |    |        |        |        |      |       |   |
|------|----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 12 | CD  | PRO | A | 16 | 5.108  | 30.911 | 11.548 | 1.00 | 50.56 | C |
| ATOM | 13 | N   | ARG | A | 17 | 7.133  | 26.746 | 10.550 | 1.00 | 48.83 | N |
| ATOM | 14 | CA  | ARG | A | 17 | 7.219  | 25.695 | 9.550  | 1.00 | 48.33 | C |
| ATOM | 15 | C   | ARG | A | 17 | 5.967  | 24.832 | 9.561  | 1.00 | 47.48 | C |
| ATOM | 16 | O   | ARG | A | 17 | 5.245  | 24.782 | 10.557 | 1.00 | 47.64 | O |
| ATOM | 17 | CB  | ARG | A | 17 | 8.421  | 24.798 | 9.835  | 1.00 | 48.61 | C |
| ATOM | 18 | CG  | ARG | A | 17 | 9.776  | 25.511 | 9.835  | 1.00 | 49.21 | C |
| ATOM | 19 | CD  | ARG | A | 17 | 10.944 | 24.577 | 10.196 | 1.00 | 49.84 | C |
| ATOM | 20 | NE  | ARG | A | 17 | 10.918 | 24.137 | 11.596 | 1.00 | 50.12 | N |
| ATOM | 21 | CZ  | ARG | A | 17 | 11.455 | 24.809 | 12.623 | 1.00 | 50.99 | C |
| ATOM | 22 | NH1 | ARG | A | 17 | 12.065 | 25.979 | 12.431 | 1.00 | 50.40 | N |
| ATOM | 23 | NH2 | ARG | A | 17 | 11.381 | 24.310 | 13.857 | 1.00 | 50.81 | N |
| ATOM | 24 | N   | GLU | A | 18 | 5.723  | 24.153 | 8.446  | 1.00 | 46.05 | N |
| ATOM | 25 | CA  | GLU | A | 18 | 4.603  | 23.246 | 8.329  | 1.00 | 45.06 | C |
| ATOM | 26 | C   | GLU | A | 18 | 5.096  | 21.830 | 8.607  | 1.00 | 44.00 | C |
| ATOM | 27 | O   | GLU | A | 18 | 6.101  | 21.405 | 8.044  | 1.00 | 43.89 | O |
| ATOM | 28 | CB  | GLU | A | 18 | 4.013  | 23.324 | 6.923  | 1.00 | 45.21 | C |
| ATOM | 29 | CG  | GLU | A | 18 | 3.323  | 24.648 | 6.621  | 1.00 | 45.56 | C |
| ATOM | 30 | CD  | GLU | A | 18 | 1.951  | 24.780 | 7.265  | 1.00 | 45.64 | C |
| ATOM | 31 | OE1 | GLU | A | 18 | 1.342  | 23.749 | 7.641  | 1.00 | 44.14 | O |
| ATOM | 32 | OE2 | GLU | A | 18 | 1.480  | 25.932 | 7.388  | 1.00 | 45.83 | O |
| ATOM | 33 | N   | GLU | A | 19 | 4.396  | 21.113 | 9.484  | 1.00 | 42.49 | N |
| ATOM | 34 | CA  | GLU | A | 19 | 4.734  | 19.728 | 9.795  | 1.00 | 41.55 | C |
| ATOM | 35 | C   | GLU | A | 19 | 4.357  | 18.817 | 8.635  | 1.00 | 39.79 | C |
| ATOM | 36 | O   | GLU | A | 19 | 3.266  | 18.933 | 8.066  | 1.00 | 39.13 | O |
| ATOM | 37 | CB  | GLU | A | 19 | 4.010  | 19.256 | 11.052 | 1.00 | 41.88 | C |
| ATOM | 38 | CG  | GLU | A | 19 | 4.420  | 19.997 | 12.311 | 1.00 | 44.80 | C |
| ATOM | 39 | CD  | GLU | A | 19 | 4.276  | 19.155 | 13.574 | 1.00 | 49.28 | C |
| ATOM | 40 | OE1 | GLU | A | 19 | 3.759  | 18.008 | 13.497 | 1.00 | 51.52 | O |
| ATOM | 41 | OE2 | GLU | A | 19 | 4.695  | 19.643 | 14.656 | 1.00 | 52.76 | O |
| ATOM | 42 | N   | ALA | A | 20 | 5.270  | 17.910 | 8.311  | 1.00 | 38.00 | N |
| ATOM | 43 | CA  | ALA | A | 20 | 5.099  | 16.952 | 7.227  | 1.00 | 36.77 | C |
| ATOM | 44 | C   | ALA | A | 20 | 3.803  | 16.168 | 7.373  | 1.00 | 35.56 | C |
| ATOM | 45 | O   | ALA | A | 20 | 3.445  | 15.734 | 8.460  | 1.00 | 35.74 | O |
| ATOM | 46 | CB  | ALA | A | 20 | 6.283  | 15.999 | 7.180  | 1.00 | 36.63 | C |
| ATOM | 47 | N   | GLY | A | 21 | 3.082  | 16.020 | 6.279  | 1.00 | 34.05 | N |
| ATOM | 48 | CA  | GLY | A | 21 | 1.860  | 15.242 | 6.307  | 1.00 | 33.24 | C |
| ATOM | 49 | C   | GLY | A | 21 | 0.666  | 16.137 | 6.551  | 1.00 | 32.36 | C |
| ATOM | 50 | O   | GLY | A | 21 | -0.393 | 15.673 | 6.951  | 1.00 | 30.93 | O |
| ATOM | 51 | N   | ALA | A | 22 | 0.867  | 17.432 | 6.323  | 1.00 | 32.41 | N |
| ATOM | 52 | CA  | ALA | A | 22 | -0.184 | 18.425 | 6.459  | 1.00 | 32.78 | C |
| ATOM | 53 | C   | ALA | A | 22 | -0.723 | 18.441 | 7.873  | 1.00 | 33.14 | C |
| ATOM | 54 | O   | ALA | A | 22 | -1.915 | 18.605 | 8.088  | 1.00 | 32.74 | O |
| ATOM | 55 | CB  | ALA | A | 22 | -1.304 | 18.139 | 5.462  | 1.00 | 32.61 | C |
| ATOM | 56 | N   | LEU | A | 23 | 0.151  | 18.253 | 8.849  | 1.00 | 34.01 | N |
| ATOM | 57 | CA  | LEU | A | 23 | -0.297 | 18.275 | 10.232 | 1.00 | 34.91 | C |
| ATOM | 58 | C   | LEU | A | 23 | -0.342 | 19.694 | 10.757 | 1.00 | 35.27 | C |
| ATOM | 59 | O   | LEU | A | 23 | -0.528 | 19.918 | 11.943 | 1.00 | 35.72 | O |
| ATOM | 60 | CB  | LEU | A | 23 | 0.565  | 17.366 | 11.097 | 1.00 | 35.27 | C |
| ATOM | 61 | CG  | LEU | A | 23 | 0.384  | 15.910 | 10.653 | 1.00 | 36.36 | C |
| ATOM | 62 | CD1 | LEU | A | 23 | 1.211  | 14.947 | 11.491 | 1.00 | 37.75 | C |
| ATOM | 63 | CD2 | LEU | A | 23 | -1.077 | 15.523 | 10.719 | 1.00 | 37.98 | C |
| ATOM | 64 | N   | GLY | A | 24 | -0.177 | 20.656 | 9.855  | 1.00 | 35.73 | N |
| ATOM | 65 | CA  | GLY | A | 24 | -0.332 | 22.053 | 10.194 | 1.00 | 35.66 | C |
| ATOM | 66 | C   | GLY | A | 24 | 0.901  | 22.655 | 10.804 | 1.00 | 36.08 | C |
| ATOM | 67 | O   | GLY | A | 24 | 1.945  | 22.001 | 10.913 | 1.00 | 36.05 | O |
| ATOM | 68 | N   | PRO | A | 25 | 0.764  | 23.894 | 11.253 | 1.00 | 35.96 | N |
| ATOM | 69 | CA  | PRO | A | 25 | 1.896  | 24.628 | 11.804 | 1.00 | 36.12 | C |
| ATOM | 70 | C   | PRO | A | 25 | 2.327  | 23.980 | 13.108 | 1.00 | 36.32 | C |
| ATOM | 71 | O   | PRO | A | 25 | 1.488  | 23.577 | 13.914 | 1.00 | 36.08 | O |
| ATOM | 72 | CB  | PRO | A | 25 | 1.341  | 26.047 | 12.043 | 1.00 | 36.15 | C |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 73  | CG  | PRO | A | 25 | -0.162 | 25.942 | 11.982 | 1.00 | 35.84 | C |
| ATOM | 74  | CD  | PRO | A | 25 | -0.504 | 24.638 | 11.350 | 1.00 | 36.22 | C |
| ATOM | 75  | N   | ALA | A | 26 | 3.632  | 23.848 | 13.285 | 1.00 | 36.64 | N |
| ATOM | 76  | CA  | ALA | A | 26 | 4.178  | 23.274 | 14.499 | 1.00 | 37.19 | C |
| ATOM | 77  | C   | ALA | A | 26 | 3.860  | 24.172 | 15.706 | 1.00 | 36.77 | C |
| ATOM | 78  | O   | ALA | A | 26 | 3.595  | 23.678 | 16.808 | 1.00 | 37.19 | O |
| ATOM | 79  | CB  | ALA | A | 26 | 5.672  | 23.099 | 14.347 | 1.00 | 37.52 | C |
| ATOM | 80  | N   | TRP | A | 27 | 3.848  | 25.479 | 15.484 | 1.00 | 35.62 | N |
| ATOM | 81  | CA  | TRP | A | 27 | 3.520  | 26.420 | 16.543 | 1.00 | 35.04 | C |
| ATOM | 82  | C   | TRP | A | 27 | 3.029  | 27.729 | 15.933 | 1.00 | 34.20 | C |
| ATOM | 83  | O   | TRP | A | 27 | 2.992  | 27.883 | 14.723 | 1.00 | 33.57 | O |
| ATOM | 84  | CB  | TRP | A | 27 | 4.774  | 26.672 | 17.382 | 1.00 | 35.28 | C |
| ATOM | 85  | CG  | TRP | A | 27 | 5.951  | 26.889 | 16.511 | 1.00 | 34.67 | C |
| ATOM | 86  | CD1 | TRP | A | 27 | 6.761  | 25.930 | 15.955 | 1.00 | 35.52 | C |
| ATOM | 87  | CD2 | TRP | A | 27 | 6.426  | 28.135 | 16.033 | 1.00 | 34.40 | C |
| ATOM | 88  | NE1 | TRP | A | 27 | 7.723  | 26.522 | 15.172 | 1.00 | 35.09 | N |
| ATOM | 89  | CE2 | TRP | A | 27 | 7.541  | 27.877 | 15.209 | 1.00 | 34.23 | C |
| ATOM | 90  | CE3 | TRP | A | 27 | 6.038  | 29.452 | 16.232 | 1.00 | 34.31 | C |
| ATOM | 91  | CZ2 | TRP | A | 27 | 8.255  | 28.879 | 14.592 | 1.00 | 35.79 | C |
| ATOM | 92  | CZ3 | TRP | A | 27 | 6.750  | 30.442 | 15.629 | 1.00 | 36.35 | C |
| ATOM | 93  | CH2 | TRP | A | 27 | 7.847  | 30.154 | 14.808 | 1.00 | 36.47 | C |
| ATOM | 94  | N   | ASP | A | 28 | 2.638  | 28.672 | 16.766 | 1.00 | 33.77 | N |
| ATOM | 95  | CA  | ASP | A | 28 | 2.259  | 29.970 | 16.249 | 1.00 | 33.48 | C |
| ATOM | 96  | C   | ASP | A | 28 | 2.759  | 31.050 | 17.165 | 1.00 | 32.26 | C |
| ATOM | 97  | O   | ASP | A | 28 | 3.210  | 30.791 | 18.276 | 1.00 | 32.05 | O |
| ATOM | 98  | CB  | ASP | A | 28 | 0.749  | 30.080 | 16.037 | 1.00 | 34.30 | C |
| ATOM | 99  | CG  | ASP | A | 28 | -0.026 | 29.986 | 17.317 | 1.00 | 36.29 | C |
| ATOM | 100 | OD1 | ASP | A | 28 | -0.184 | 31.027 | 18.002 | 1.00 | 39.59 | O |
| ATOM | 101 | OD2 | ASP | A | 28 | -0.517 | 28.906 | 17.712 | 1.00 | 39.78 | O |
| ATOM | 102 | N   | GLU | A | 29 | 2.691  | 32.268 | 16.654 | 1.00 | 31.30 | N |
| ATOM | 103 | CA  | GLU | A | 29 | 3.181  | 33.465 | 17.326 | 1.00 | 30.15 | C |
| ATOM | 104 | C   | GLU | A | 29 | 2.674  | 33.625 | 18.752 | 1.00 | 28.85 | C |
| ATOM | 105 | O   | GLU | A | 29 | 3.407  | 34.036 | 19.621 | 1.00 | 28.58 | O |
| ATOM | 106 | CB  | GLU | A | 29 | 2.791  | 34.682 | 16.503 | 1.00 | 30.32 | C |
| ATOM | 107 | N   | SER | A | 30 | 1.414  | 33.313 | 18.992 | 1.00 | 27.95 | N |
| ATOM | 108 | CA  | SER | A | 30 | 0.845  | 33.501 | 20.320 | 1.00 | 27.46 | C |
| ATOM | 109 | C   | SER | A | 30 | 1.537  | 32.671 | 21.389 | 1.00 | 26.93 | C |
| ATOM | 110 | O   | SER | A | 30 | 1.312  | 32.907 | 22.567 | 1.00 | 26.79 | O |
| ATOM | 111 | CB  | SER | A | 30 | -0.651 | 33.168 | 20.322 | 1.00 | 27.23 | C |
| ATOM | 112 | OG  | SER | A | 30 | -0.857 | 31.764 | 20.306 | 1.00 | 27.69 | O |
| ATOM | 113 | N   | GLN | A | 31 | 2.360  | 31.703 | 20.984 | 1.00 | 26.55 | N |
| ATOM | 114 | CA  | GLN | A | 31 | 3.071  | 30.837 | 21.926 | 1.00 | 26.63 | C |
| ATOM | 115 | C   | GLN | A | 31 | 4.419  | 31.409 | 22.334 | 1.00 | 26.66 | C |
| ATOM | 116 | O   | GLN | A | 31 | 5.078  | 30.855 | 23.205 | 1.00 | 26.45 | O |
| ATOM | 117 | CB  | GLN | A | 31 | 3.282  | 29.426 | 21.349 | 1.00 | 26.41 | C |
| ATOM | 118 | CG  | GLN | A | 31 | 1.998  | 28.637 | 21.131 | 1.00 | 26.28 | C |
| ATOM | 119 | CD  | GLN | A | 31 | 2.245  | 27.287 | 20.489 | 1.00 | 26.25 | C |
| ATOM | 120 | OE1 | GLN | A | 31 | 2.258  | 27.183 | 19.271 | 1.00 | 27.92 | O |
| ATOM | 121 | NE2 | GLN | A | 31 | 2.465  | 26.258 | 21.305 | 1.00 | 24.36 | N |
| ATOM | 122 | N   | LEU | A | 32 | 4.824  | 32.508 | 21.703 | 1.00 | 26.89 | N |
| ATOM | 123 | CA  | LEU | A | 32 | 6.083  | 33.176 | 22.029 | 1.00 | 27.24 | C |
| ATOM | 124 | C   | LEU | A | 32 | 5.852  | 34.321 | 23.006 | 1.00 | 26.92 | C |
| ATOM | 125 | O   | LEU | A | 32 | 4.888  | 35.047 | 22.868 | 1.00 | 26.42 | O |
| ATOM | 126 | CB  | LEU | A | 32 | 6.717  | 33.746 | 20.760 | 1.00 | 27.46 | C |
| ATOM | 127 | CG  | LEU | A | 32 | 6.964  | 32.728 | 19.640 | 1.00 | 28.65 | C |
| ATOM | 128 | CD1 | LEU | A | 32 | 7.630  | 33.391 | 18.452 | 1.00 | 29.44 | C |
| ATOM | 129 | CD2 | LEU | A | 32 | 7.792  | 31.573 | 20.127 | 1.00 | 27.98 | C |
| ATOM | 130 | N   | ARG | A | 33 | 6.728  | 34.472 | 23.995 | 1.00 | 26.71 | N |
| ATOM | 131 | CA  | ARG | A | 33 | 6.627  | 35.596 | 24.923 | 1.00 | 26.77 | C |
| ATOM | 132 | C   | ARG | A | 33 | 7.040  | 36.880 | 24.209 | 1.00 | 26.57 | C |
| ATOM | 133 | O   | ARG | A | 33 | 7.719  | 36.844 | 23.203 | 1.00 | 26.30 | O |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 134 | CB  | ARG | A | 33 | 7.492  | 35.357 | 26.163 | 1.00 | 26.67 | C |
| ATOM | 135 | CG  | ARG | A | 33 | 7.052  | 34.141 | 26.983 | 1.00 | 26.29 | C |
| ATOM | 136 | CD  | ARG | A | 33 | 7.937  | 33.837 | 28.181 | 1.00 | 25.85 | C |
| ATOM | 137 | NE  | ARG | A | 33 | 7.381  | 32.778 | 29.018 | 1.00 | 25.80 | N |
| ATOM | 138 | CZ  | ARG | A | 33 | 6.451  | 32.946 | 29.945 | 1.00 | 24.68 | C |
| ATOM | 139 | NH1 | ARG | A | 33 | 5.937  | 34.140 | 30.189 | 1.00 | 23.50 | N |
| ATOM | 140 | NH2 | ARG | A | 33 | 6.029  | 31.901 | 30.637 | 1.00 | 25.35 | N |
| ATOM | 141 | N   | SER | A | 34 | 6.633  | 38.020 | 24.732 | 1.00 | 26.80 | N |
| ATOM | 142 | CA  | SER | A | 34 | 6.903  | 39.280 | 24.061 | 1.00 | 27.15 | C |
| ATOM | 143 | C   | SER | A | 34 | 7.990  | 40.048 | 24.791 | 1.00 | 26.39 | C |
| ATOM | 144 | O   | SER | A | 34 | 7.964  | 40.140 | 26.005 | 1.00 | 25.87 | O |
| ATOM | 145 | CB  | SER | A | 34 | 5.628  | 40.104 | 24.030 | 1.00 | 27.68 | C |
| ATOM | 146 | OG  | SER | A | 34 | 5.494  | 40.737 | 25.285 | 1.00 | 32.47 | O |
| ATOM | 147 | N   | TYR | A | 35 | 8.944  | 40.589 | 24.042 | 1.00 | 25.89 | N |
| ATOM | 148 | CA  | TYR | A | 35 | 10.110 | 41.223 | 24.637 | 1.00 | 26.28 | C |
| ATOM | 149 | C   | TYR | A | 35 | 10.353 | 42.558 | 23.970 | 1.00 | 26.85 | C |
| ATOM | 150 | O   | TYR | A | 35 | 9.722  | 42.856 | 22.967 | 1.00 | 26.92 | O |
| ATOM | 151 | CB  | TYR | A | 35 | 11.326 | 40.308 | 24.510 | 1.00 | 25.90 | C |
| ATOM | 152 | CG  | TYR | A | 35 | 11.169 | 39.032 | 25.309 | 1.00 | 25.33 | C |
| ATOM | 153 | CD1 | TYR | A | 35 | 10.975 | 39.073 | 26.685 | 1.00 | 24.99 | C |
| ATOM | 154 | CD2 | TYR | A | 35 | 11.198 | 37.787 | 24.692 | 1.00 | 23.82 | C |
| ATOM | 155 | CE1 | TYR | A | 35 | 10.823 | 37.898 | 27.429 | 1.00 | 24.56 | C |
| ATOM | 156 | CE2 | TYR | A | 35 | 11.046 | 36.620 | 25.426 | 1.00 | 24.42 | C |
| ATOM | 157 | CZ  | TYR | A | 35 | 10.862 | 36.682 | 26.793 | 1.00 | 23.48 | C |
| ATOM | 158 | OH  | TYR | A | 35 | 10.696 | 35.524 | 27.513 | 1.00 | 24.75 | O |
| ATOM | 159 | N   | SER | A | 36 | 11.304 | 43.327 | 24.496 | 1.00 | 27.27 | N |
| ATOM | 160 | CA  | SER | A | 36 | 11.525 | 44.704 | 24.052 | 1.00 | 27.55 | C |
| ATOM | 161 | C   | SER | A | 36 | 12.513 | 44.912 | 22.917 | 1.00 | 27.06 | C |
| ATOM | 162 | O   | SER | A | 36 | 12.734 | 46.049 | 22.504 | 1.00 | 27.94 | O |
| ATOM | 163 | CB  | SER | A | 36 | 12.082 | 45.498 | 25.226 | 1.00 | 27.88 | C |
| ATOM | 164 | OG  | SER | A | 36 | 13.350 | 44.976 | 25.590 | 1.00 | 28.36 | O |
| ATOM | 165 | N   | PHE | A | 37 | 13.128 | 43.851 | 22.429 | 1.00 | 25.35 | N |
| ATOM | 166 | CA  | PHE | A | 37 | 14.202 | 44.014 | 21.461 | 1.00 | 24.62 | C |
| ATOM | 167 | C   | PHE | A | 37 | 13.899 | 43.272 | 20.159 | 1.00 | 24.75 | C |
| ATOM | 168 | O   | PHE | A | 37 | 13.130 | 42.335 | 20.135 | 1.00 | 24.25 | O |
| ATOM | 169 | CB  | PHE | A | 37 | 15.487 | 43.462 | 22.071 | 1.00 | 23.87 | C |
| ATOM | 170 | CG  | PHE | A | 37 | 15.318 | 42.069 | 22.635 | 1.00 | 22.53 | C |
| ATOM | 171 | CD1 | PHE | A | 37 | 15.348 | 40.972 | 21.802 | 1.00 | 21.11 | C |
| ATOM | 172 | CD2 | PHE | A | 37 | 15.069 | 41.872 | 23.988 | 1.00 | 21.63 | C |
| ATOM | 173 | CE1 | PHE | A | 37 | 15.158 | 39.687 | 22.314 | 1.00 | 22.41 | C |
| ATOM | 174 | CE2 | PHE | A | 37 | 14.900 | 40.612 | 24.505 | 1.00 | 22.29 | C |
| ATOM | 175 | CZ  | PHE | A | 37 | 14.936 | 39.509 | 23.675 | 1.00 | 21.45 | C |
| ATOM | 176 | N   | PRO | A | 38 | 14.489 | 43.715 | 19.067 | 1.00 | 24.94 | N |
| ATOM | 177 | CA  | PRO | A | 38 | 14.322 | 43.017 | 17.793 | 1.00 | 24.67 | C |
| ATOM | 178 | C   | PRO | A | 38 | 15.267 | 41.823 | 17.678 | 1.00 | 24.41 | C |
| ATOM | 179 | O   | PRO | A | 38 | 16.249 | 41.745 | 18.427 | 1.00 | 23.73 | O |
| ATOM | 180 | CB  | PRO | A | 38 | 14.725 | 44.072 | 16.783 | 1.00 | 24.75 | C |
| ATOM | 181 | CG  | PRO | A | 38 | 15.791 | 44.872 | 17.530 | 1.00 | 26.09 | C |
| ATOM | 182 | CD  | PRO | A | 38 | 15.287 | 44.950 | 18.941 | 1.00 | 25.27 | C |
| ATOM | 183 | N   | THR | A | 39 | 14.981 | 40.927 | 16.734 | 1.00 | 23.30 | N |
| ATOM | 184 | CA  | THR | A | 39 | 15.859 | 39.816 | 16.444 | 1.00 | 23.42 | C |
| ATOM | 185 | C   | THR | A | 39 | 15.857 | 39.534 | 14.955 | 1.00 | 24.29 | C |
| ATOM | 186 | O   | THR | A | 39 | 14.958 | 39.964 | 14.239 | 1.00 | 24.61 | O |
| ATOM | 187 | CB  | THR | A | 39 | 15.368 | 38.538 | 17.135 | 1.00 | 23.09 | C |
| ATOM | 188 | OG1 | THR | A | 39 | 14.044 | 38.232 | 16.680 | 1.00 | 19.92 | O |
| ATOM | 189 | CG2 | THR | A | 39 | 15.213 | 38.731 | 18.641 | 1.00 | 23.03 | C |
| ATOM | 190 | N   | ARG | A | 40 | 16.854 | 38.773 | 14.525 | 1.00 | 24.43 | N |
| ATOM | 191 | CA  | ARG | A | 40 | 16.982 | 38.273 | 13.170 | 1.00 | 24.91 | C |
| ATOM | 192 | C   | ARG | A | 40 | 17.061 | 36.751 | 13.268 | 1.00 | 24.49 | C |
| ATOM | 193 | O   | ARG | A | 40 | 17.434 | 36.225 | 14.301 | 1.00 | 23.58 | O |
| ATOM | 194 | CB  | ARG | A | 40 | 18.253 | 38.805 | 12.536 | 1.00 | 25.36 | C |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 195 | CG  | ARG | A | 40 | 18.208 | 40.281 | 12.248 | 1.00 | 30.74 | C |
| ATOM | 196 | CD  | ARG | A | 40 | 16.823 | 40.775 | 11.890 | 1.00 | 34.86 | C |
| ATOM | 197 | NE  | ARG | A | 40 | 16.604 | 40.989 | 10.477 | 1.00 | 39.38 | N |
| ATOM | 198 | CZ  | ARG | A | 40 | 15.403 | 41.229 | 9.971  | 1.00 | 43.86 | C |
| ATOM | 199 | NH1 | ARG | A | 40 | 14.345 | 41.254 | 10.782 | 1.00 | 45.88 | N |
| ATOM | 200 | NH2 | ARG | A | 40 | 15.252 | 41.457 | 8.674  | 1.00 | 44.96 | N |
| ATOM | 201 | N   | PRO | A | 41 | 16.687 | 36.031 | 12.221 | 1.00 | 25.08 | N |
| ATOM | 202 | CA  | PRO | A | 41 | 16.715 | 34.565 | 12.290 | 1.00 | 25.39 | C |
| ATOM | 203 | C   | PRO | A | 41 | 18.095 | 33.913 | 12.282 | 1.00 | 25.10 | C |
| ATOM | 204 | O   | PRO | A | 41 | 19.007 | 34.370 | 11.636 | 1.00 | 25.16 | O |
| ATOM | 205 | CB  | PRO | A | 41 | 15.953 | 34.130 | 11.023 | 1.00 | 25.76 | C |
| ATOM | 206 | CG  | PRO | A | 41 | 15.286 | 35.392 | 10.504 | 1.00 | 26.54 | C |
| ATOM | 207 | CD  | PRO | A | 41 | 16.151 | 36.524 | 10.939 | 1.00 | 24.85 | C |
| ATOM | 208 | N   | ILE | A | 42 | 18.225 | 32.823 | 13.020 | 1.00 | 25.28 | N |
| ATOM | 209 | CA  | ILE | A | 42 | 19.388 | 31.974 | 12.919 | 1.00 | 24.31 | C |
| ATOM | 210 | C   | ILE | A | 42 | 19.147 | 31.116 | 11.677 | 1.00 | 24.68 | C |
| ATOM | 211 | O   | ILE | A | 42 | 18.043 | 30.614 | 11.466 | 1.00 | 24.72 | O |
| ATOM | 212 | CB  | ILE | A | 42 | 19.481 | 31.104 | 14.163 | 1.00 | 24.80 | C |
| ATOM | 213 | CG1 | ILE | A | 42 | 19.763 | 31.993 | 15.384 | 1.00 | 24.24 | C |
| ATOM | 214 | CG2 | ILE | A | 42 | 20.530 | 30.004 | 13.961 | 1.00 | 23.81 | C |
| ATOM | 215 | CD1 | ILE | A | 42 | 19.531 | 31.325 | 16.729 | 1.00 | 23.59 | C |
| ATOM | 216 | N   | PRO | A | 43 | 20.146 | 30.953 | 10.826 | 1.00 | 24.48 | N |
| ATOM | 217 | CA  | PRO | A | 43 | 19.963 | 30.108 | 9.651  | 1.00 | 24.60 | C |
| ATOM | 218 | C   | PRO | A | 43 | 19.611 | 28.650 | 10.001 | 1.00 | 24.85 | C |
| ATOM | 219 | O   | PRO | A | 43 | 20.148 | 28.130 | 10.989 | 1.00 | 24.38 | O |
| ATOM | 220 | CB  | PRO | A | 43 | 21.320 | 30.192 | 8.937  | 1.00 | 24.87 | C |
| ATOM | 221 | CG  | PRO | A | 43 | 22.040 | 31.372 | 9.541  | 1.00 | 25.04 | C |
| ATOM | 222 | CD  | PRO | A | 43 | 21.475 | 31.583 | 10.886 | 1.00 | 24.37 | C |
| ATOM | 223 | N   | ARG | A | 44 | 18.686 | 28.032 | 9.248  | 1.00 | 24.70 | N |
| ATOM | 224 | CA  | ARG | A | 44 | 18.367 | 26.608 | 9.391  | 1.00 | 25.53 | C |
| ATOM | 225 | C   | ARG | A | 44 | 18.910 | 25.943 | 8.152  | 1.00 | 25.00 | C |
| ATOM | 226 | O   | ARG | A | 44 | 18.505 | 26.265 | 7.030  | 1.00 | 24.62 | O |
| ATOM | 227 | CB  | ARG | A | 44 | 16.873 | 26.287 | 9.452  | 1.00 | 26.51 | C |
| ATOM | 228 | CG  | ARG | A | 44 | 16.044 | 27.133 | 10.378 | 1.00 | 29.49 | C |
| ATOM | 229 | CD  | ARG | A | 44 | 14.683 | 26.485 | 10.813 | 1.00 | 31.03 | C |
| ATOM | 230 | NE  | ARG | A | 44 | 14.401 | 25.120 | 10.323 | 1.00 | 32.36 | N |
| ATOM | 231 | CZ  | ARG | A | 44 | 14.174 | 24.057 | 11.126 | 1.00 | 33.85 | C |
| ATOM | 232 | NH1 | ARG | A | 44 | 14.239 | 24.170 | 12.451 | 1.00 | 30.71 | N |
| ATOM | 233 | NH2 | ARG | A | 44 | 13.898 | 22.863 | 10.613 | 1.00 | 35.56 | N |
| ATOM | 234 | N   | LEU | A | 45 | 19.815 | 25.006 | 8.337  | 1.00 | 23.91 | N |
| ATOM | 235 | CA  | LEU | A | 45 | 20.500 | 24.444 | 7.202  | 1.00 | 23.40 | C |
| ATOM | 236 | C   | LEU | A | 45 | 20.684 | 22.967 | 7.352  | 1.00 | 23.52 | C |
| ATOM | 237 | O   | LEU | A | 45 | 20.559 | 22.423 | 8.446  | 1.00 | 22.50 | O |
| ATOM | 238 | CB  | LEU | A | 45 | 21.888 | 25.064 | 7.093  | 1.00 | 22.62 | C |
| ATOM | 239 | CG  | LEU | A | 45 | 21.911 | 26.563 | 6.819  | 1.00 | 23.96 | C |
| ATOM | 240 | CD1 | LEU | A | 45 | 23.317 | 27.111 | 6.947  | 1.00 | 24.52 | C |
| ATOM | 241 | CD2 | LEU | A | 45 | 21.366 | 26.845 | 5.423  | 1.00 | 24.63 | C |
| ATOM | 242 | N   | SER | A | 46 | 21.018 | 22.347 | 6.227  | 1.00 | 23.57 | N |
| ATOM | 243 | CA  | SER | A | 46 | 21.382 | 20.975 | 6.221  | 1.00 | 24.12 | C |
| ATOM | 244 | C   | SER | A | 46 | 22.820 | 20.888 | 6.668  | 1.00 | 24.81 | C |
| ATOM | 245 | O   | SER | A | 46 | 23.640 | 21.757 | 6.398  | 1.00 | 23.76 | O |
| ATOM | 246 | CB  | SER | A | 46 | 21.236 | 20.354 | 4.830  | 1.00 | 23.80 | C |
| ATOM | 247 | OG  | SER | A | 46 | 21.744 | 19.020 | 4.830  | 1.00 | 24.09 | O |
| ATOM | 248 | N   | GLN | A | 47 | 23.089 | 19.804 | 7.366  | 1.00 | 25.92 | N |
| ATOM | 249 | CA  | GLN | A | 47 | 24.399 | 19.444 | 7.844  | 1.00 | 27.25 | C |
| ATOM | 250 | C   | GLN | A | 47 | 25.379 | 19.326 | 6.674  | 1.00 | 27.54 | C |
| ATOM | 251 | O   | GLN | A | 47 | 26.563 | 19.564 | 6.836  | 1.00 | 27.97 | O |
| ATOM | 252 | CB  | GLN | A | 47 | 24.245 | 18.088 | 8.554  | 1.00 | 28.46 | C |
| ATOM | 253 | CG  | GLN | A | 47 | 25.487 | 17.279 | 8.705  | 1.00 | 31.10 | C |
| ATOM | 254 | CD  | GLN | A | 47 | 25.776 | 16.372 | 7.570  | 1.00 | 33.17 | C |
| ATOM | 255 | OE1 | GLN | A | 47 | 24.881 | 15.970 | 6.803  | 1.00 | 36.23 | O |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 256 | NE2 | GLN | A | 47 | 27.041 | 16.000 | 7.458  | 1.00 | 36.17 | N |
| ATOM | 257 | N   | SER | A | 48 | 24.884 | 18.951 | 5.498  | 1.00 | 27.72 | N |
| ATOM | 258 | CA  | SER | A | 48 | 25.736 | 18.809 | 4.323  | 1.00 | 28.35 | C |
| ATOM | 259 | C   | SER | A | 48 | 26.016 | 20.150 | 3.629  | 1.00 | 28.86 | C |
| ATOM | 260 | O   | SER | A | 48 | 26.825 | 20.235 | 2.711  | 1.00 | 28.96 | O |
| ATOM | 261 | CB  | SER | A | 48 | 25.092 | 17.839 | 3.324  | 1.00 | 28.65 | C |
| ATOM | 262 | OG  | SER | A | 48 | 23.798 | 18.276 | 2.918  | 1.00 | 28.51 | O |
| ATOM | 263 | N   | ASP | A | 49 | 25.347 | 21.203 | 4.065  | 1.00 | 29.16 | N |
| ATOM | 264 | CA  | ASP | A | 49 | 25.515 | 22.496 | 3.442  | 1.00 | 29.28 | C |
| ATOM | 265 | C   | ASP | A | 49 | 26.800 | 23.163 | 3.913  | 1.00 | 29.71 | C |
| ATOM | 266 | O   | ASP | A | 49 | 26.981 | 23.398 | 5.101  | 1.00 | 29.02 | O |
| ATOM | 267 | CB  | ASP | A | 49 | 24.325 | 23.369 | 3.783  | 1.00 | 29.35 | C |
| ATOM | 268 | CG  | ASP | A | 49 | 24.316 | 24.667 | 3.010  | 1.00 | 29.93 | C |
| ATOM | 269 | OD1 | ASP | A | 49 | 25.398 | 25.183 | 2.666  | 1.00 | 28.14 | O |
| ATOM | 270 | OD2 | ASP | A | 49 | 23.259 | 25.247 | 2.731  | 1.00 | 30.49 | O |
| ATOM | 271 | N   | PRO | A | 50 | 27.693 | 23.483 | 2.976  | 1.00 | 30.34 | N |
| ATOM | 272 | CA  | PRO | A | 50 | 28.964 | 24.134 | 3.315  | 1.00 | 30.54 | C |
| ATOM | 273 | C   | PRO | A | 50 | 28.783 | 25.354 | 4.186  | 1.00 | 30.38 | C |
| ATOM | 274 | O   | PRO | A | 50 | 29.661 | 25.651 | 4.990  | 1.00 | 30.53 | O |
| ATOM | 275 | CB  | PRO | A | 50 | 29.520 | 24.573 | 1.952  | 1.00 | 30.39 | C |
| ATOM | 276 | CG  | PRO | A | 50 | 28.926 | 23.667 | 0.988  | 1.00 | 30.96 | C |
| ATOM | 277 | CD  | PRO | A | 50 | 27.574 | 23.243 | 1.531  | 1.00 | 30.51 | C |
| ATOM | 278 | N   | ARG | A | 51 | 27.683 | 26.072 | 4.008  | 1.00 | 30.50 | N |
| ATOM | 279 | CA  | ARG | A | 51 | 27.439 | 27.253 | 4.817  | 1.00 | 30.94 | C |
| ATOM | 280 | C   | ARG | A | 51 | 27.341 | 26.875 | 6.299  | 1.00 | 30.49 | C |
| ATOM | 281 | O   | ARG | A | 51 | 27.744 | 27.646 | 7.161  | 1.00 | 29.74 | O |
| ATOM | 282 | CB  | ARG | A | 51 | 26.171 | 27.979 | 4.370  | 1.00 | 30.97 | C |
| ATOM | 283 | CG  | ARG | A | 51 | 26.337 | 28.781 | 3.099  | 1.00 | 33.47 | C |
| ATOM | 284 | CD  | ARG | A | 51 | 25.029 | 29.321 | 2.521  | 1.00 | 34.80 | C |
| ATOM | 285 | NE  | ARG | A | 51 | 24.071 | 28.252 | 2.221  | 1.00 | 36.68 | N |
| ATOM | 286 | CZ  | ARG | A | 51 | 22.766 | 28.448 | 2.081  | 1.00 | 37.94 | C |
| ATOM | 287 | NH1 | ARG | A | 51 | 22.260 | 29.677 | 2.208  | 1.00 | 39.10 | N |
| ATOM | 288 | NH2 | ARG | A | 51 | 21.967 | 27.436 | 1.794  | 1.00 | 36.51 | N |
| ATOM | 289 | N   | ALA | A | 52 | 26.831 | 25.684 | 6.596  | 1.00 | 30.03 | N |
| ATOM | 290 | CA  | ALA | A | 52 | 26.697 | 25.288 | 7.993  | 1.00 | 29.96 | C |
| ATOM | 291 | C   | ALA | A | 52 | 28.079 | 25.101 | 8.593  | 1.00 | 30.07 | C |
| ATOM | 292 | O   | ALA | A | 52 | 28.345 | 25.518 | 9.710  | 1.00 | 29.00 | O |
| ATOM | 293 | CB  | ALA | A | 52 | 25.901 | 24.028 | 8.119  | 1.00 | 29.81 | C |
| ATOM | 294 | N   | GLU | A | 53 | 28.958 | 24.455 | 7.845  | 1.00 | 30.12 | N |
| ATOM | 295 | CA  | GLU | A | 53 | 30.290 | 24.213 | 8.347  | 1.00 | 31.08 | C |
| ATOM | 296 | C   | GLU | A | 53 | 30.999 | 25.550 | 8.579  | 1.00 | 30.37 | C |
| ATOM | 297 | O   | GLU | A | 53 | 31.683 | 25.730 | 9.580  | 1.00 | 29.89 | O |
| ATOM | 298 | CB  | GLU | A | 53 | 31.086 | 23.362 | 7.379  | 1.00 | 31.41 | C |
| ATOM | 299 | CG  | GLU | A | 53 | 32.189 | 22.603 | 8.081  | 1.00 | 35.02 | C |
| ATOM | 300 | CD  | GLU | A | 53 | 31.785 | 21.185 | 8.507  | 1.00 | 37.87 | C |
| ATOM | 301 | OE1 | GLU | A | 53 | 30.614 | 20.929 | 8.887  | 1.00 | 39.16 | O |
| ATOM | 302 | OE2 | GLU | A | 53 | 32.674 | 20.313 | 8.463  | 1.00 | 40.43 | O |
| ATOM | 303 | N   | GLU | A | 54 | 30.811 | 26.479 | 7.652  | 1.00 | 29.84 | N |
| ATOM | 304 | CA  | GLU | A | 54 | 31.413 | 27.796 | 7.757  | 1.00 | 30.22 | C |
| ATOM | 305 | C   | GLU | A | 54 | 30.975 | 28.486 | 9.045  | 1.00 | 29.05 | C |
| ATOM | 306 | O   | GLU | A | 54 | 31.780 | 29.102 | 9.719  | 1.00 | 28.03 | O |
| ATOM | 307 | CB  | GLU | A | 54 | 31.026 | 28.680 | 6.573  | 1.00 | 30.53 | C |
| ATOM | 308 | CG  | GLU | A | 54 | 31.635 | 28.276 | 5.243  | 1.00 | 34.66 | C |
| ATOM | 309 | CD  | GLU | A | 54 | 30.993 | 29.002 | 4.058  | 1.00 | 38.49 | C |
| ATOM | 310 | OE1 | GLU | A | 54 | 30.651 | 30.208 | 4.214  | 1.00 | 42.20 | O |
| ATOM | 311 | OE2 | GLU | A | 54 | 30.829 | 28.368 | 2.975  | 1.00 | 41.54 | O |
| ATOM | 312 | N   | LEU | A | 55 | 29.696 | 28.366 | 9.387  | 1.00 | 28.24 | N |
| ATOM | 313 | CA  | LEU | A | 55 | 29.177 | 29.029 | 10.571 | 1.00 | 27.28 | C |
| ATOM | 314 | C   | LEU | A | 55 | 29.774 | 28.448 | 11.827 | 1.00 | 26.43 | C |
| ATOM | 315 | O   | LEU | A | 55 | 30.212 | 29.199 | 12.695 | 1.00 | 25.20 | O |
| ATOM | 316 | CB  | LEU | A | 55 | 27.655 | 28.975 | 10.597 | 1.00 | 27.25 | C |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 317 | CG  | LEU | A | 55 | 27.027 | 29.829 | 9.502  | 1.00 | 27.43 | C |
| ATOM | 318 | CD1 | LEU | A | 55 | 25.568 | 29.452 | 9.322  | 1.00 | 28.83 | C |
| ATOM | 319 | CD2 | LEU | A | 55 | 27.173 | 31.318 | 9.821  | 1.00 | 26.98 | C |
| ATOM | 320 | N   | ILE | A | 56 | 29.829 | 27.116 | 11.915 | 1.00 | 25.75 | N |
| ATOM | 321 | CA  | ILE | A | 56 | 30.382 | 26.473 | 13.107 | 1.00 | 25.50 | C |
| ATOM | 322 | C   | ILE | A | 56 | 31.874 | 26.815 | 13.254 | 1.00 | 26.26 | C |
| ATOM | 323 | O   | ILE | A | 56 | 32.346 | 27.134 | 14.349 | 1.00 | 25.55 | O |
| ATOM | 324 | CB  | ILE | A | 56 | 30.192 | 24.955 | 13.059 | 1.00 | 25.63 | C |
| ATOM | 325 | CG1 | ILE | A | 56 | 28.698 | 24.574 | 13.034 | 1.00 | 24.00 | C |
| ATOM | 326 | CG2 | ILE | A | 56 | 30.848 | 24.321 | 14.263 | 1.00 | 25.48 | C |
| ATOM | 327 | CD1 | ILE | A | 56 | 28.439 | 23.170 | 12.531 | 1.00 | 24.10 | C |
| ATOM | 328 | N   | GLU | A | 57 | 32.597 | 26.781 | 12.135 | 1.00 | 27.04 | N |
| ATOM | 329 | CA  | GLU | A | 57 | 34.023 | 27.082 | 12.107 | 1.00 | 28.01 | C |
| ATOM | 330 | C   | GLU | A | 57 | 34.232 | 28.491 | 12.625 | 1.00 | 28.49 | C |
| ATOM | 331 | O   | GLU | A | 57 | 35.183 | 28.770 | 13.344 | 1.00 | 28.92 | O |
| ATOM | 332 | CB  | GLU | A | 57 | 34.561 | 26.977 | 10.676 | 1.00 | 28.61 | C |
| ATOM | 333 | CG  | GLU | A | 57 | 36.053 | 27.224 | 10.509 | 1.00 | 30.77 | C |
| ATOM | 334 | CD  | GLU | A | 57 | 36.902 | 26.322 | 11.394 | 1.00 | 35.15 | C |
| ATOM | 335 | OE1 | GLU | A | 57 | 36.556 | 25.127 | 11.591 | 1.00 | 37.11 | O |
| ATOM | 336 | OE2 | GLU | A | 57 | 37.924 | 26.818 | 11.909 | 1.00 | 40.88 | O |
| ATOM | 337 | N   | ASN | A | 58 | 33.321 | 29.378 | 12.270 | 1.00 | 28.34 | N |
| ATOM | 338 | CA  | ASN | A | 58 | 33.424 | 30.758 | 12.701 | 1.00 | 28.81 | C |
| ATOM | 339 | C   | ASN | A | 58 | 32.770 | 31.079 | 14.025 | 1.00 | 27.23 | C |
| ATOM | 340 | O   | ASN | A | 58 | 32.630 | 32.233 | 14.374 | 1.00 | 26.07 | O |
| ATOM | 341 | CB  | ASN | A | 58 | 32.792 | 31.641 | 11.656 | 1.00 | 29.66 | C |
| ATOM | 342 | CG  | ASN | A | 58 | 33.789 | 32.386 | 10.913 | 1.00 | 33.61 | C |
| ATOM | 343 | OD1 | ASN | A | 58 | 34.280 | 31.901 | 9.893  | 1.00 | 38.81 | O |
| ATOM | 344 | ND2 | ASN | A | 58 | 34.160 | 33.582 | 11.429 | 1.00 | 36.72 | N |
| ATOM | 345 | N   | GLU | A | 59 | 32.343 | 30.053 | 14.735 | 1.00 | 26.39 | N |
| ATOM | 346 | CA  | GLU | A | 59 | 31.712 | 30.241 | 16.030 | 1.00 | 26.36 | C |
| ATOM | 347 | C   | GLU | A | 59 | 30.495 | 31.144 | 15.926 | 1.00 | 25.39 | C |
| ATOM | 348 | O   | GLU | A | 59 | 30.325 | 32.100 | 16.668 | 1.00 | 24.14 | O |
| ATOM | 349 | CB  | GLU | A | 59 | 32.753 | 30.697 | 17.059 | 1.00 | 26.80 | C |
| ATOM | 350 | CG  | GLU | A | 59 | 33.717 | 29.537 | 17.316 | 1.00 | 29.10 | C |
| ATOM | 351 | CD  | GLU | A | 59 | 34.722 | 29.791 | 18.407 | 1.00 | 32.85 | C |
| ATOM | 352 | OE1 | GLU | A | 59 | 35.790 | 30.330 | 18.080 | 1.00 | 37.47 | O |
| ATOM | 353 | OE2 | GLU | A | 59 | 34.466 | 29.432 | 19.572 | 1.00 | 34.14 | O |
| ATOM | 354 | N   | GLU | A | 60 | 29.641 | 30.799 | 14.970 | 1.00 | 24.88 | N |
| ATOM | 355 | CA  | GLU | A | 60 | 28.366 | 31.465 | 14.801 | 1.00 | 25.20 | C |
| ATOM | 356 | C   | GLU | A | 60 | 27.262 | 30.414 | 14.822 | 1.00 | 24.07 | C |
| ATOM | 357 | O   | GLU | A | 60 | 27.420 | 29.320 | 14.293 | 1.00 | 22.49 | O |
| ATOM | 358 | CB  | GLU | A | 60 | 28.343 | 32.249 | 13.505 | 1.00 | 25.69 | C |
| ATOM | 359 | CG  | GLU | A | 60 | 29.354 | 33.363 | 13.536 | 1.00 | 30.40 | C |
| ATOM | 360 | CD  | GLU | A | 60 | 28.962 | 34.516 | 12.657 | 1.00 | 37.91 | C |
| ATOM | 361 | OE1 | GLU | A | 60 | 29.009 | 34.377 | 11.414 | 1.00 | 38.24 | O |
| ATOM | 362 | OE2 | GLU | A | 60 | 28.595 | 35.566 | 13.236 | 1.00 | 46.50 | O |
| ATOM | 363 | N   | PRO | A | 61 | 26.124 | 30.779 | 15.386 | 1.00 | 22.90 | N |
| ATOM | 364 | CA  | PRO | A | 61 | 25.045 | 29.816 | 15.571 | 1.00 | 22.19 | C |
| ATOM | 365 | C   | PRO | A | 61 | 24.448 | 29.371 | 14.267 | 1.00 | 21.47 | C |
| ATOM | 366 | O   | PRO | A | 61 | 24.419 | 30.104 | 13.266 | 1.00 | 20.48 | O |
| ATOM | 367 | CB  | PRO | A | 61 | 23.996 | 30.583 | 16.368 | 1.00 | 22.29 | C |
| ATOM | 368 | CG  | PRO | A | 61 | 24.315 | 32.053 | 16.148 | 1.00 | 22.67 | C |
| ATOM | 369 | CD  | PRO | A | 61 | 25.764 | 32.140 | 15.798 | 1.00 | 22.92 | C |
| ATOM | 370 | N   | VAL | A | 62 | 23.957 | 28.142 | 14.283 | 1.00 | 20.87 | N |
| ATOM | 371 | CA  | VAL | A | 62 | 23.248 | 27.591 | 13.146 | 1.00 | 20.94 | C |
| ATOM | 372 | C   | VAL | A | 62 | 22.353 | 26.475 | 13.655 | 1.00 | 21.15 | C |
| ATOM | 373 | O   | VAL | A | 62 | 22.714 | 25.761 | 14.605 | 1.00 | 21.21 | O |
| ATOM | 374 | CB  | VAL | A | 62 | 24.214 | 27.052 | 12.073 | 1.00 | 21.30 | C |
| ATOM | 375 | CG1 | VAL | A | 62 | 25.061 | 25.912 | 12.608 | 1.00 | 22.10 | C |
| ATOM | 376 | CG2 | VAL | A | 62 | 23.440 | 26.587 | 10.825 | 1.00 | 21.19 | C |
| ATOM | 377 | N   | VAL | A | 63 | 21.158 | 26.366 | 13.084 | 1.00 | 21.48 | N |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 378 | CA  | VAL | A | 63 | 20.302 | 25.231 | 13.374 | 1.00 | 21.87 | C |
| ATOM | 379 | C   | VAL | A | 63 | 20.526 | 24.212 | 12.270 | 1.00 | 22.00 | C |
| ATOM | 380 | O   | VAL | A | 63 | 20.366 | 24.528 | 11.109 | 1.00 | 22.54 | O |
| ATOM | 381 | CB  | VAL | A | 63 | 18.793 | 25.574 | 13.421 | 1.00 | 22.02 | C |
| ATOM | 382 | CG1 | VAL | A | 63 | 17.955 | 24.277 | 13.612 | 1.00 | 21.90 | C |
| ATOM | 383 | CG2 | VAL | A | 63 | 18.494 | 26.522 | 14.546 | 1.00 | 21.22 | C |
| ATOM | 384 | N   | LEU | A | 64 | 20.911 | 23.002 | 12.643 | 1.00 | 22.48 | N |
| ATOM | 385 | CA  | LEU | A | 64 | 21.067 | 21.902 | 11.710 | 1.00 | 23.08 | C |
| ATOM | 386 | C   | LEU | A | 64 | 19.826 | 21.014 | 11.775 | 1.00 | 22.19 | C |
| ATOM | 387 | O   | LEU | A | 64 | 19.423 | 20.558 | 12.843 | 1.00 | 21.85 | O |
| ATOM | 388 | CB  | LEU | A | 64 | 22.327 | 21.107 | 12.032 | 1.00 | 24.00 | C |
| ATOM | 389 | CG  | LEU | A | 64 | 23.614 | 21.930 | 11.984 | 1.00 | 27.02 | C |
| ATOM | 390 | CD1 | LEU | A | 64 | 24.791 | 21.080 | 12.303 | 1.00 | 31.61 | C |
| ATOM | 391 | CD2 | LEU | A | 64 | 23.827 | 22.540 | 10.640 | 1.00 | 29.86 | C |
| ATOM | 392 | N   | THR | A | 65 | 19.222 | 20.757 | 10.628 | 1.00 | 21.50 | N |
| ATOM | 393 | CA  | THR | A | 65 | 17.943 | 20.056 | 10.613 | 1.00 | 21.95 | C |
| ATOM | 394 | C   | THR | A | 65 | 18.022 | 18.561 | 10.389 | 1.00 | 21.35 | C |
| ATOM | 395 | O   | THR | A | 65 | 17.028 | 17.870 | 10.581 | 1.00 | 21.37 | O |
| ATOM | 396 | CB  | THR | A | 65 | 17.062 | 20.592 | 9.478  | 1.00 | 22.08 | C |
| ATOM | 397 | OG1 | THR | A | 65 | 17.725 | 20.351 | 8.230  | 1.00 | 22.38 | O |
| ATOM | 398 | CG2 | THR | A | 65 | 16.919 | 22.099 | 9.553  | 1.00 | 24.00 | C |
| ATOM | 399 | N   | ASP | A | 66 | 19.168 | 18.062 | 9.961  | 1.00 | 21.50 | N |
| ATOM | 400 | CA  | ASP | A | 66 | 19.259 | 16.650 | 9.604  | 1.00 | 21.86 | C |
| ATOM | 401 | C   | ASP | A | 66 | 20.513 | 15.899 | 10.069 | 1.00 | 21.61 | C |
| ATOM | 402 | O   | ASP | A | 66 | 21.070 | 15.088 | 9.316  | 1.00 | 21.82 | O |
| ATOM | 403 | CB  | ASP | A | 66 | 19.152 | 16.553 | 8.084  | 1.00 | 22.20 | C |
| ATOM | 404 | CG  | ASP | A | 66 | 20.199 | 17.355 | 7.390  | 1.00 | 21.49 | C |
| ATOM | 405 | OD1 | ASP | A | 66 | 21.065 | 17.936 | 8.070  | 1.00 | 21.14 | O |
| ATOM | 406 | OD2 | ASP | A | 66 | 20.240 | 17.477 | 6.159  | 1.00 | 25.40 | O |
| ATOM | 407 | N   | THR | A | 67 | 20.967 | 16.158 | 11.287 | 1.00 | 21.05 | N |
| ATOM | 408 | CA  | THR | A | 67 | 22.154 | 15.491 | 11.768 | 1.00 | 20.85 | C |
| ATOM | 409 | C   | THR | A | 67 | 21.858 | 14.084 | 12.231 | 1.00 | 20.12 | C |
| ATOM | 410 | O   | THR | A | 67 | 22.757 | 13.281 | 12.283 | 1.00 | 20.45 | O |
| ATOM | 411 | CB  | THR | A | 67 | 22.747 | 16.207 | 12.977 | 1.00 | 20.77 | C |
| ATOM | 412 | OG1 | THR | A | 67 | 21.782 | 16.210 | 14.039 | 1.00 | 20.61 | O |
| ATOM | 413 | CG2 | THR | A | 67 | 23.054 | 17.671 | 12.682 | 1.00 | 22.44 | C |
| ATOM | 414 | N   | ASN | A | 68 | 20.614 | 13.815 | 12.618 | 1.00 | 19.51 | N |
| ATOM | 415 | CA  | ASN | A | 68 | 20.269 | 12.555 | 13.267 | 1.00 | 19.09 | C |
| ATOM | 416 | C   | ASN | A | 68 | 21.116 | 12.349 | 14.517 | 1.00 | 18.40 | C |
| ATOM | 417 | O   | ASN | A | 68 | 21.383 | 11.212 | 14.928 | 1.00 | 17.67 | O |
| ATOM | 418 | CB  | ASN | A | 68 | 20.455 | 11.362 | 12.325 | 1.00 | 19.63 | C |
| ATOM | 419 | CG  | ASN | A | 68 | 19.453 | 11.344 | 11.209 | 1.00 | 19.93 | C |
| ATOM | 420 | OD1 | ASN | A | 68 | 18.253 | 11.236 | 11.442 | 1.00 | 19.76 | O |
| ATOM | 421 | ND2 | ASN | A | 68 | 19.941 | 11.423 | 9.987  | 1.00 | 19.96 | N |
| ATOM | 422 | N   | LEU | A | 69 | 21.532 | 13.448 | 15.134 | 1.00 | 18.28 | N |
| ATOM | 423 | CA  | LEU | A | 69 | 22.378 | 13.382 | 16.326 | 1.00 | 17.98 | C |
| ATOM | 424 | C   | LEU | A | 69 | 21.773 | 12.542 | 17.447 | 1.00 | 17.59 | C |
| ATOM | 425 | O   | LEU | A | 69 | 22.478 | 11.725 | 18.039 | 1.00 | 17.61 | O |
| ATOM | 426 | CB  | LEU | A | 69 | 22.693 | 14.772 | 16.844 | 1.00 | 18.38 | C |
| ATOM | 427 | CG  | LEU | A | 69 | 23.636 | 14.859 | 18.035 | 1.00 | 18.31 | C |
| ATOM | 428 | CD1 | LEU | A | 69 | 24.936 | 14.144 | 17.744 | 1.00 | 20.68 | C |
| ATOM | 429 | CD2 | LEU | A | 69 | 23.907 | 16.299 | 18.399 | 1.00 | 19.25 | C |
| ATOM | 430 | N   | VAL | A | 70 | 20.489 | 12.741 | 17.740 | 1.00 | 17.27 | N |
| ATOM | 431 | CA  | VAL | A | 70 | 19.811 | 11.989 | 18.794 | 1.00 | 17.72 | C |
| ATOM | 432 | C   | VAL | A | 70 | 18.588 | 11.253 | 18.257 | 1.00 | 18.11 | C |
| ATOM | 433 | O   | VAL | A | 70 | 17.557 | 11.148 | 18.927 | 1.00 | 17.23 | O |
| ATOM | 434 | CB  | VAL | A | 70 | 19.395 | 12.866 | 19.999 | 1.00 | 17.54 | C |
| ATOM | 435 | CG1 | VAL | A | 70 | 20.624 | 13.402 | 20.704 | 1.00 | 19.07 | C |
| ATOM | 436 | CG2 | VAL | A | 70 | 18.451 | 13.994 | 19.599 | 1.00 | 17.50 | C |
| ATOM | 437 | N   | TYR | A | 71 | 18.715 | 10.764 | 17.028 | 1.00 | 19.22 | N |
| ATOM | 438 | CA  | TYR | A | 71 | 17.615 | 10.071 | 16.367 | 1.00 | 19.79 | C |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 439 | C   | TYR | A | 71 | 16.934 | 9.072  | 17.306 | 1.00 | 19.62 | C |
| ATOM | 440 | O   | TYR | A | 71 | 15.726 | 9.120  | 17.457 | 1.00 | 18.64 | O |
| ATOM | 441 | CB  | TYR | A | 71 | 18.082 | 9.406  | 15.055 | 1.00 | 20.19 | C |
| ATOM | 442 | CG  | TYR | A | 71 | 17.156 | 8.320  | 14.554 | 1.00 | 22.29 | C |
| ATOM | 443 | CD1 | TYR | A | 71 | 15.938 | 8.619  | 13.948 | 1.00 | 25.33 | C |
| ATOM | 444 | CD2 | TYR | A | 71 | 17.503 | 6.986  | 14.691 | 1.00 | 23.31 | C |
| ATOM | 445 | CE1 | TYR | A | 71 | 15.080 | 7.555  | 13.480 | 1.00 | 24.74 | C |
| ATOM | 446 | CE2 | TYR | A | 71 | 16.684 | 5.968  | 14.252 | 1.00 | 23.57 | C |
| ATOM | 447 | CZ  | TYR | A | 71 | 15.479 | 6.244  | 13.650 | 1.00 | 24.07 | C |
| ATOM | 448 | OH  | TYR | A | 71 | 14.686 | 5.159  | 13.266 | 1.00 | 27.86 | O |
| ATOM | 449 | N   | PRO | A | 72 | 17.688 | 8.200  | 17.960 | 1.00 | 20.27 | N |
| ATOM | 450 | CA  | PRO | A | 72 | 17.074 | 7.196  | 18.840 | 1.00 | 21.30 | C |
| ATOM | 451 | C   | PRO | A | 72 | 16.307 | 7.794  | 20.008 | 1.00 | 21.82 | C |
| ATOM | 452 | O   | PRO | A | 72 | 15.463 | 7.120  | 20.535 | 1.00 | 21.13 | O |
| ATOM | 453 | CB  | PRO | A | 72 | 18.267 | 6.377  | 19.351 | 1.00 | 21.33 | C |
| ATOM | 454 | CG  | PRO | A | 72 | 19.362 | 6.650  | 18.386 | 1.00 | 21.75 | C |
| ATOM | 455 | CD  | PRO | A | 72 | 19.151 | 8.065  | 17.905 | 1.00 | 20.71 | C |
| ATOM | 456 | N   | ALA | A | 73 | 16.588 | 9.038  | 20.391 | 1.00 | 22.47 | N |
| ATOM | 457 | CA  | ALA | A | 73 | 15.892 | 9.658  | 21.522 | 1.00 | 23.20 | C |
| ATOM | 458 | C   | ALA | A | 73 | 14.567 | 10.293 | 21.103 | 1.00 | 23.47 | C |
| ATOM | 459 | O   | ALA | A | 73 | 13.801 | 10.765 | 21.938 | 1.00 | 23.46 | O |
| ATOM | 460 | CB  | ALA | A | 73 | 16.783 | 10.718 | 22.173 | 1.00 | 23.27 | C |
| ATOM | 461 | N   | LEU | A | 74 | 14.297 | 10.322 | 19.808 | 1.00 | 23.79 | N |
| ATOM | 462 | CA  | LEU | A | 74 | 13.086 | 10.967 | 19.329 | 1.00 | 24.10 | C |
| ATOM | 463 | C   | LEU | A | 74 | 11.797 | 10.301 | 19.801 | 1.00 | 24.55 | C |
| ATOM | 464 | O   | LEU | A | 74 | 10.732 | 10.903 | 19.746 | 1.00 | 23.83 | O |
| ATOM | 465 | CB  | LEU | A | 74 | 13.114 | 11.076 | 17.810 | 1.00 | 24.16 | C |
| ATOM | 466 | CG  | LEU | A | 74 | 14.185 | 12.061 | 17.296 | 1.00 | 24.67 | C |
| ATOM | 467 | CD1 | LEU | A | 74 | 13.988 | 12.320 | 15.820 | 1.00 | 26.73 | C |
| ATOM | 468 | CD2 | LEU | A | 74 | 14.225 | 13.371 | 18.077 | 1.00 | 23.39 | C |
| ATOM | 469 | N   | LYS | A | 75 | 11.897 | 9.053  | 20.244 | 1.00 | 24.97 | N |
| ATOM | 470 | CA  | LYS | A | 75 | 10.741 | 8.317  | 20.738 | 1.00 | 25.16 | C |
| ATOM | 471 | C   | LYS | A | 75 | 10.589 | 8.519  | 22.245 | 1.00 | 25.37 | C |
| ATOM | 472 | O   | LYS | A | 75 | 9.612  | 8.082  | 22.822 | 1.00 | 25.23 | O |
| ATOM | 473 | CB  | LYS | A | 75 | 10.885 | 6.819  | 20.428 | 1.00 | 25.16 | C |
| ATOM | 474 | CG  | LYS | A | 75 | 12.079 | 6.163  | 21.097 | 1.00 | 25.17 | C |
| ATOM | 475 | CD  | LYS | A | 75 | 12.178 | 4.653  | 20.765 | 1.00 | 27.19 | C |
| ATOM | 476 | CE  | LYS | A | 75 | 13.646 | 4.220  | 20.609 | 1.00 | 26.95 | C |
| ATOM | 477 | NZ  | LYS | A | 75 | 14.348 | 4.123  | 21.868 | 1.00 | 26.22 | N |
| ATOM | 478 | N   | TRP | A | 76 | 11.552 | 9.179  | 22.882 | 1.00 | 25.25 | N |
| ATOM | 479 | CA  | TRP | A | 76 | 11.486 | 9.389  | 24.319 | 1.00 | 25.56 | C |
| ATOM | 480 | C   | TRP | A | 76 | 10.268 | 10.201 | 24.749 | 1.00 | 26.35 | C |
| ATOM | 481 | O   | TRP | A | 76 | 9.920  | 11.198 | 24.130 | 1.00 | 26.71 | O |
| ATOM | 482 | CB  | TRP | A | 76 | 12.719 | 10.139 | 24.816 | 1.00 | 25.19 | C |
| ATOM | 483 | CG  | TRP | A | 76 | 13.975 | 9.338  | 24.816 | 1.00 | 24.32 | C |
| ATOM | 484 | CD1 | TRP | A | 76 | 14.129 | 8.059  | 24.393 | 1.00 | 22.72 | C |
| ATOM | 485 | CD2 | TRP | A | 76 | 15.258 | 9.762  | 25.271 | 1.00 | 22.34 | C |
| ATOM | 486 | NE1 | TRP | A | 76 | 15.431 | 7.658  | 24.552 | 1.00 | 20.61 | N |
| ATOM | 487 | CE2 | TRP | A | 76 | 16.145 | 8.685  | 25.096 | 1.00 | 20.28 | C |
| ATOM | 488 | CE3 | TRP | A | 76 | 15.750 | 10.944 | 25.817 | 1.00 | 22.65 | C |
| ATOM | 489 | CZ2 | TRP | A | 76 | 17.481 | 8.756  | 25.437 | 1.00 | 20.18 | C |
| ATOM | 490 | CZ3 | TRP | A | 76 | 17.088 | 11.012 | 26.163 | 1.00 | 21.43 | C |
| ATOM | 491 | CH2 | TRP | A | 76 | 17.932 | 9.934  | 25.970 | 1.00 | 21.94 | C |
| ATOM | 492 | N   | ASP | A | 77 | 9.643  | 9.772  | 25.836 | 1.00 | 26.46 | N |
| ATOM | 493 | CA  | ASP | A | 77 | 8.583  | 10.530 | 26.467 | 1.00 | 26.47 | C |
| ATOM | 494 | C   | ASP | A | 77 | 8.618  | 10.116 | 27.931 | 1.00 | 26.16 | C |
| ATOM | 495 | O   | ASP | A | 77 | 9.405  | 9.264  | 28.291 | 1.00 | 26.44 | O |
| ATOM | 496 | CB  | ASP | A | 77 | 7.230  | 10.276 | 25.810 | 1.00 | 26.51 | C |
| ATOM | 497 | CG  | ASP | A | 77 | 6.795  | 8.835  | 25.885 | 1.00 | 27.32 | C |
| ATOM | 498 | OD1 | ASP | A | 77 | 7.388  | 8.015  | 26.638 | 1.00 | 26.02 | O |
| ATOM | 499 | OD2 | ASP | A | 77 | 5.832  | 8.439  | 25.211 | 1.00 | 29.97 | O |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 500 | N   | LEU | A | 78 | 7.790  | 10.705 | 28.775 | 1.00 | 25.96 | N |
| ATOM | 501 | CA  | LEU | A | 78 | 7.893  | 10.441 | 30.201 | 1.00 | 26.27 | C |
| ATOM | 502 | C   | LEU | A | 78 | 7.716  | 8.965  | 30.539 | 1.00 | 26.14 | C |
| ATOM | 503 | O   | LEU | A | 78 | 8.446  | 8.438  | 31.374 | 1.00 | 25.51 | O |
| ATOM | 504 | CB  | LEU | A | 78 | 6.905  | 11.301 | 30.979 | 1.00 | 26.32 | C |
| ATOM | 505 | CG  | LEU | A | 78 | 7.155  | 12.802 | 30.860 | 1.00 | 27.35 | C |
| ATOM | 506 | CD1 | LEU | A | 78 | 6.098  | 13.579 | 31.623 | 1.00 | 28.05 | C |
| ATOM | 507 | CD2 | LEU | A | 78 | 8.536  | 13.165 | 31.379 | 1.00 | 28.39 | C |
| ATOM | 508 | N   | GLU | A | 79 | 6.775  | 8.297  | 29.874 | 1.00 | 26.56 | N |
| ATOM | 509 | CA  | GLU | A | 79 | 6.526  | 6.876  | 30.123 | 1.00 | 27.00 | C |
| ATOM | 510 | C   | GLU | A | 79 | 7.754  | 6.029  | 29.780 | 1.00 | 26.63 | C |
| ATOM | 511 | O   | GLU | A | 79 | 8.220  | 5.231  | 30.583 | 1.00 | 25.94 | O |
| ATOM | 512 | CB  | GLU | A | 79 | 5.302  | 6.371  | 29.333 | 1.00 | 27.39 | C |
| ATOM | 513 | CG  | GLU | A | 79 | 4.963  | 4.919  | 29.657 | 1.00 | 29.75 | C |
| ATOM | 514 | CD  | GLU | A | 79 | 3.803  | 4.347  | 28.854 | 1.00 | 33.15 | C |
| ATOM | 515 | OE1 | GLU | A | 79 | 3.361  | 4.976  | 27.863 | 1.00 | 35.39 | O |
| ATOM | 516 | OE2 | GLU | A | 79 | 3.338  | 3.245  | 29.224 | 1.00 | 35.44 | O |
| ATOM | 517 | N   | TYR | A | 80 | 8.279  | 6.205  | 28.575 | 1.00 | 26.53 | N |
| ATOM | 518 | CA  | TYR | A | 80 | 9.466  | 5.465  | 28.169 | 1.00 | 26.29 | C |
| ATOM | 519 | C   | TYR | A | 80 | 10.669 | 5.763  | 29.072 | 1.00 | 25.83 | C |
| ATOM | 520 | O   | TYR | A | 80 | 11.418 | 4.863  | 29.435 | 1.00 | 25.75 | O |
| ATOM | 521 | CB  | TYR | A | 80 | 9.812  | 5.802  | 26.728 | 1.00 | 26.53 | C |
| ATOM | 522 | CG  | TYR | A | 80 | 11.047 | 5.106  | 26.210 | 1.00 | 26.94 | C |
| ATOM | 523 | CD1 | TYR | A | 80 | 10.971 | 3.836  | 25.637 | 1.00 | 26.53 | C |
| ATOM | 524 | CD2 | TYR | A | 80 | 12.287 | 5.721  | 26.291 | 1.00 | 25.32 | C |
| ATOM | 525 | CE1 | TYR | A | 80 | 12.113 | 3.208  | 25.142 | 1.00 | 26.28 | C |
| ATOM | 526 | CE2 | TYR | A | 80 | 13.416 | 5.109  | 25.823 | 1.00 | 25.73 | C |
| ATOM | 527 | CZ  | TYR | A | 80 | 13.331 | 3.861  | 25.240 | 1.00 | 25.94 | C |
| ATOM | 528 | OH  | TYR | A | 80 | 14.478 | 3.294  | 24.758 | 1.00 | 25.55 | O |
| ATOM | 529 | N   | LEU | A | 81 | 10.859 | 7.016  | 29.448 | 1.00 | 25.62 | N |
| ATOM | 530 | CA  | LEU | A | 81 | 12.000 | 7.350  | 30.309 | 1.00 | 25.87 | C |
| ATOM | 531 | C   | LEU | A | 81 | 11.821 | 6.794  | 31.733 | 1.00 | 26.06 | C |
| ATOM | 532 | O   | LEU | A | 81 | 12.763 | 6.263  | 32.327 | 1.00 | 26.00 | O |
| ATOM | 533 | CB  | LEU | A | 81 | 12.250 | 8.863  | 30.340 | 1.00 | 25.81 | C |
| ATOM | 534 | CG  | LEU | A | 81 | 12.748 | 9.501  | 29.030 | 1.00 | 25.65 | C |
| ATOM | 535 | CD1 | LEU | A | 81 | 12.828 | 11.010 | 29.174 | 1.00 | 26.40 | C |
| ATOM | 536 | CD2 | LEU | A | 81 | 14.102 | 8.959  | 28.592 | 1.00 | 25.79 | C |
| ATOM | 537 | N   | GLN | A | 82 | 10.617 | 6.913  | 32.274 | 1.00 | 26.27 | N |
| ATOM | 538 | CA  | GLN | A | 82 | 10.338 | 6.388  | 33.602 | 1.00 | 26.77 | C |
| ATOM | 539 | C   | GLN | A | 82 | 10.640 | 4.897  | 33.623 | 1.00 | 26.51 | C |
| ATOM | 540 | O   | GLN | A | 82 | 11.232 | 4.384  | 34.552 | 1.00 | 26.60 | O |
| ATOM | 541 | CB  | GLN | A | 82 | 8.877  | 6.611  | 33.974 | 1.00 | 26.90 | C |
| ATOM | 542 | CG  | GLN | A | 82 | 8.466  | 5.856  | 35.236 | 1.00 | 28.41 | C |
| ATOM | 543 | CD  | GLN | A | 82 | 7.315  | 6.501  | 35.987 | 1.00 | 30.63 | C |
| ATOM | 544 | OE1 | GLN | A | 82 | 6.755  | 7.501  | 35.551 | 1.00 | 32.13 | O |
| ATOM | 545 | NE2 | GLN | A | 82 | 6.944  | 5.907  | 37.116 | 1.00 | 34.12 | N |
| ATOM | 546 | N   | GLU | A | 83 | 10.252 | 4.216  | 32.561 | 1.00 | 26.68 | N |
| ATOM | 547 | CA  | GLU | A | 83 | 10.429 | 2.773  | 32.456 | 1.00 | 26.90 | C |
| ATOM | 548 | C   | GLU | A | 83 | 11.893 | 2.359  | 32.295 | 1.00 | 26.42 | C |
| ATOM | 549 | O   | GLU | A | 83 | 12.285 | 1.294  | 32.764 | 1.00 | 25.50 | O |
| ATOM | 550 | CB  | GLU | A | 83 | 9.604  | 2.257  | 31.273 | 1.00 | 26.84 | C |
| ATOM | 551 | CG  | GLU | A | 83 | 9.607  | 0.753  | 31.080 | 1.00 | 29.20 | C |
| ATOM | 552 | CD  | GLU | A | 83 | 8.902  | 0.014  | 32.205 | 1.00 | 31.92 | C |
| ATOM | 553 | OE1 | GLU | A | 83 | 8.258  | 0.666  | 33.060 | 1.00 | 34.06 | O |
| ATOM | 554 | OE2 | GLU | A | 83 | 9.008  | -1.221 | 32.243 | 1.00 | 33.78 | O |
| ATOM | 555 | N   | ASN | A | 84 | 12.711 | 3.223  | 31.700 | 1.00 | 25.79 | N |
| ATOM | 556 | CA  | ASN | A | 84 | 14.063 | 2.824  | 31.312 | 1.00 | 25.87 | C |
| ATOM | 557 | C   | ASN | A | 84 | 15.273 | 3.607  | 31.810 | 1.00 | 26.08 | C |
| ATOM | 558 | O   | ASN | A | 84 | 16.392 | 3.138  | 31.628 | 1.00 | 26.05 | O |
| ATOM | 559 | CB  | ASN | A | 84 | 14.137 | 2.844  | 29.784 | 1.00 | 25.74 | C |
| ATOM | 560 | CG  | ASN | A | 84 | 13.262 | 1.799  | 29.152 | 1.00 | 25.67 | C |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 561 | OD1 | ASN | A | 84 | 13.402 | 0.608  | 29.439 | 1.00 | 24.26 | O |
| ATOM | 562 | ND2 | ASN | A | 84 | 12.354 | 2.231  | 28.288 | 1.00 | 22.66 | N |
| ATOM | 563 | N   | ILE | A | 85 | 15.087 | 4.773  | 32.422 | 1.00 | 26.02 | N |
| ATOM | 564 | CA  | ILE | A | 85 | 16.240 | 5.599  | 32.763 | 1.00 | 26.74 | C |
| ATOM | 565 | C   | ILE | A | 85 | 16.930 | 5.307  | 34.099 | 1.00 | 26.89 | C |
| ATOM | 566 | O   | ILE | A | 85 | 17.820 | 6.054  | 34.519 | 1.00 | 26.93 | O |
| ATOM | 567 | CB  | ILE | A | 85 | 15.846 | 7.076  | 32.688 | 1.00 | 26.70 | C |
| ATOM | 568 | CG1 | ILE | A | 85 | 17.049 | 7.923  | 32.270 | 1.00 | 27.99 | C |
| ATOM | 569 | CG2 | ILE | A | 85 | 15.232 | 7.535  | 33.988 | 1.00 | 26.50 | C |
| ATOM | 570 | CD1 | ILE | A | 85 | 16.696 | 9.389  | 32.000 | 1.00 | 28.77 | C |
| ATOM | 571 | N   | GLY | A | 86 | 16.503 | 4.253  | 34.773 | 1.00 | 27.27 | N |
| ATOM | 572 | CA  | GLY | A | 86 | 17.130 | 3.834  | 36.018 | 1.00 | 27.51 | C |
| ATOM | 573 | C   | GLY | A | 86 | 16.573 | 4.453  | 37.289 | 1.00 | 27.73 | C |
| ATOM | 574 | O   | GLY | A | 86 | 15.563 | 5.163  | 37.268 | 1.00 | 27.80 | O |
| ATOM | 575 | N   | ASN | A | 87 | 17.273 | 4.186  | 38.392 | 1.00 | 27.70 | N |
| ATOM | 576 | CA  | ASN | A | 87 | 16.864 | 4.603  | 39.726 | 1.00 | 27.53 | C |
| ATOM | 577 | C   | ASN | A | 87 | 17.849 | 5.602  | 40.320 | 1.00 | 27.33 | C |
| ATOM | 578 | O   | ASN | A | 87 | 17.932 | 5.762  | 41.539 | 1.00 | 26.97 | O |
| ATOM | 579 | CB  | ASN | A | 87 | 16.726 | 3.367  | 40.644 | 1.00 | 27.60 | C |
| ATOM | 580 | N   | GLY | A | 88 | 18.601 | 6.273  | 39.455 | 1.00 | 27.41 | N |
| ATOM | 581 | CA  | GLY | A | 88 | 19.528 | 7.307  | 39.888 | 1.00 | 27.29 | C |
| ATOM | 582 | C   | GLY | A | 88 | 18.762 | 8.549  | 40.288 | 1.00 | 27.18 | C |
| ATOM | 583 | O   | GLY | A | 88 | 17.570 | 8.654  | 40.001 | 1.00 | 27.43 | O |
| ATOM | 584 | N   | ASP | A | 89 | 19.437 | 9.489  | 40.945 | 1.00 | 27.04 | N |
| ATOM | 585 | CA  | ASP | A | 89 | 18.808 | 10.739 | 41.366 | 1.00 | 26.88 | C |
| ATOM | 586 | C   | ASP | A | 89 | 18.761 | 11.755 | 40.227 | 1.00 | 26.69 | C |
| ATOM | 587 | O   | ASP | A | 89 | 19.697 | 11.848 | 39.446 | 1.00 | 26.91 | O |
| ATOM | 588 | CB  | ASP | A | 89 | 19.596 | 11.372 | 42.504 | 1.00 | 26.95 | C |
| ATOM | 589 | CG  | ASP | A | 89 | 19.375 | 10.688 | 43.834 | 1.00 | 27.28 | C |
| ATOM | 590 | OD1 | ASP | A | 89 | 18.499 | 9.811  | 43.939 | 1.00 | 29.31 | O |
| ATOM | 591 | OD2 | ASP | A | 89 | 20.040 | 10.983 | 44.839 | 1.00 | 27.32 | O |
| ATOM | 592 | N   | PHE | A | 90 | 17.687 | 12.531 | 40.152 | 1.00 | 26.24 | N |
| ATOM | 593 | CA  | PHE | A | 90 | 17.598 | 13.594 | 39.165 | 1.00 | 26.10 | C |
| ATOM | 594 | C   | PHE | A | 90 | 17.407 | 14.931 | 39.866 | 1.00 | 26.23 | C |
| ATOM | 595 | O   | PHE | A | 90 | 16.629 | 15.037 | 40.811 | 1.00 | 26.48 | O |
| ATOM | 596 | CB  | PHE | A | 90 | 16.460 | 13.322 | 38.184 | 1.00 | 25.91 | C |
| ATOM | 597 | CG  | PHE | A | 90 | 16.747 | 12.201 | 37.241 | 1.00 | 25.26 | C |
| ATOM | 598 | CD1 | PHE | A | 90 | 16.601 | 10.886 | 37.640 | 1.00 | 25.32 | C |
| ATOM | 599 | CD2 | PHE | A | 90 | 17.190 | 12.459 | 35.958 | 1.00 | 26.02 | C |
| ATOM | 600 | CE1 | PHE | A | 90 | 16.872 | 9.856  | 36.777 | 1.00 | 24.09 | C |
| ATOM | 601 | CE2 | PHE | A | 90 | 17.460 | 11.427 | 35.091 | 1.00 | 25.07 | C |
| ATOM | 602 | CZ  | PHE | A | 90 | 17.308 | 10.117 | 35.512 | 1.00 | 24.67 | C |
| ATOM | 603 | N   | SER | A | 91 | 18.149 | 15.941 | 39.430 | 1.00 | 26.33 | N |
| ATOM | 604 | CA  | SER | A | 91 | 17.985 | 17.280 | 39.973 | 1.00 | 26.48 | C |
| ATOM | 605 | C   | SER | A | 91 | 16.777 | 17.923 | 39.310 | 1.00 | 26.71 | C |
| ATOM | 606 | O   | SER | A | 91 | 16.696 | 18.029 | 38.077 | 1.00 | 26.09 | O |
| ATOM | 607 | CB  | SER | A | 91 | 19.226 | 18.152 | 39.763 | 1.00 | 26.25 | C |
| ATOM | 608 | OG  | SER | A | 91 | 20.364 | 17.543 | 40.326 | 1.00 | 26.61 | O |
| ATOM | 609 | N   | VAL | A | 92 | 15.835 | 18.327 | 40.150 | 1.00 | 27.06 | N |
| ATOM | 610 | CA  | VAL | A | 92 | 14.629 | 18.971 | 39.695 | 1.00 | 27.44 | C |
| ATOM | 611 | C   | VAL | A | 92 | 14.468 | 20.295 | 40.405 | 1.00 | 27.57 | C |
| ATOM | 612 | O   | VAL | A | 92 | 14.475 | 20.376 | 41.642 | 1.00 | 26.69 | O |
| ATOM | 613 | CB  | VAL | A | 92 | 13.407 | 18.132 | 40.004 | 1.00 | 27.60 | C |
| ATOM | 614 | CG1 | VAL | A | 92 | 12.164 | 18.800 | 39.432 | 1.00 | 28.15 | C |
| ATOM | 615 | CG2 | VAL | A | 92 | 13.584 | 16.731 | 39.457 | 1.00 | 27.84 | C |
| ATOM | 616 | N   | TYR | A | 93 | 14.312 | 21.334 | 39.598 | 1.00 | 27.77 | N |
| ATOM | 617 | CA  | TYR | A | 93 | 14.120 | 22.661 | 40.108 | 1.00 | 27.91 | C |
| ATOM | 618 | C   | TYR | A | 93 | 12.654 | 22.940 | 40.172 | 1.00 | 28.16 | C |
| ATOM | 619 | O   | TYR | A | 93 | 11.894 | 22.525 | 39.303 | 1.00 | 28.02 | O |
| ATOM | 620 | CB  | TYR | A | 93 | 14.810 | 23.673 | 39.216 | 1.00 | 27.94 | C |
| ATOM | 621 | CG  | TYR | A | 93 | 16.291 | 23.593 | 39.368 | 1.00 | 29.53 | C |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 622 | CD1 | TYR | A | 93  | 16.929 | 24.258 | 40.395 | 1.00 | 29.48 | C |
| ATOM | 623 | CD2 | TYR | A | 93  | 17.046 | 22.815 | 38.522 | 1.00 | 30.95 | C |
| ATOM | 624 | CE1 | TYR | A | 93  | 18.266 | 24.169 | 40.553 | 1.00 | 29.93 | C |
| ATOM | 625 | CE2 | TYR | A | 93  | 18.386 | 22.726 | 38.679 | 1.00 | 31.90 | C |
| ATOM | 626 | CZ  | TYR | A | 93  | 18.985 | 23.402 | 39.704 | 1.00 | 31.56 | C |
| ATOM | 627 | OH  | TYR | A | 93  | 20.327 | 23.306 | 39.878 | 1.00 | 35.47 | O |
| ATOM | 628 | N   | SER | A | 94  | 12.282 | 23.669 | 41.208 | 1.00 | 28.70 | N |
| ATOM | 629 | CA  | SER | A | 94  | 10.913 | 24.037 | 41.459 | 1.00 | 29.47 | C |
| ATOM | 630 | C   | SER | A | 94  | 10.856 | 25.547 | 41.554 | 1.00 | 29.69 | C |
| ATOM | 631 | O   | SER | A | 94  | 11.705 | 26.167 | 42.187 | 1.00 | 29.50 | O |
| ATOM | 632 | CB  | SER | A | 94  | 10.456 | 23.411 | 42.774 | 1.00 | 29.32 | C |
| ATOM | 633 | OG  | SER | A | 94  | 9.093  | 23.701 | 43.009 | 1.00 | 30.85 | O |
| ATOM | 634 | N   | ALA | A | 95  | 9.858  | 26.146 | 40.928 | 1.00 | 30.39 | N |
| ATOM | 635 | CA  | ALA | A | 95  | 9.760  | 27.591 | 40.929 | 1.00 | 31.04 | C |
| ATOM | 636 | C   | ALA | A | 95  | 8.330  | 28.064 | 40.932 | 1.00 | 31.76 | C |
| ATOM | 637 | O   | ALA | A | 95  | 7.425  | 27.386 | 40.452 | 1.00 | 31.87 | O |
| ATOM | 638 | CB  | ALA | A | 95  | 10.480 | 28.165 | 39.716 | 1.00 | 31.12 | C |
| ATOM | 639 | N   | SER | A | 96  | 8.147  | 29.258 | 41.467 | 1.00 | 32.54 | N |
| ATOM | 640 | CA  | SER | A | 96  | 6.848  | 29.891 | 41.489 | 1.00 | 33.42 | C |
| ATOM | 641 | C   | SER | A | 96  | 6.708  | 30.869 | 40.326 | 1.00 | 33.15 | C |
| ATOM | 642 | O   | SER | A | 96  | 5.662  | 31.487 | 40.163 | 1.00 | 34.35 | O |
| ATOM | 643 | CB  | SER | A | 96  | 6.673  | 30.661 | 42.787 | 1.00 | 33.88 | C |
| ATOM | 644 | OG  | SER | A | 96  | 5.380  | 31.217 | 42.815 | 1.00 | 35.79 | O |
| ATOM | 645 | N   | THR | A | 97  | 7.775  | 31.031 | 39.554 | 1.00 | 32.09 | N |
| ATOM | 646 | CA  | THR | A | 97  | 7.797  | 31.920 | 38.397 | 1.00 | 31.44 | C |
| ATOM | 647 | C   | THR | A | 97  | 8.185  | 31.095 | 37.191 | 1.00 | 30.26 | C |
| ATOM | 648 | O   | THR | A | 97  | 8.693  | 30.003 | 37.348 | 1.00 | 29.72 | O |
| ATOM | 649 | CB  | THR | A | 97  | 8.857  | 33.031 | 38.582 | 1.00 | 31.64 | C |
| ATOM | 650 | OG1 | THR | A | 97  | 9.147  | 33.656 | 37.323 | 1.00 | 32.17 | O |
| ATOM | 651 | CG2 | THR | A | 97  | 10.227 | 32.455 | 38.978 | 1.00 | 31.73 | C |
| ATOM | 652 | N   | HIS | A | 98  | 7.974  | 31.623 | 35.996 | 1.00 | 29.35 | N |
| ATOM | 653 | CA  | HIS | A | 98  | 8.379  | 30.915 | 34.780 | 1.00 | 28.83 | C |
| ATOM | 654 | C   | HIS | A | 98  | 9.899  | 30.969 | 34.589 | 1.00 | 28.37 | C |
| ATOM | 655 | O   | HIS | A | 98  | 10.467 | 30.189 | 33.824 | 1.00 | 27.53 | O |
| ATOM | 656 | CB  | HIS | A | 98  | 7.671  | 31.490 | 33.548 | 1.00 | 28.76 | C |
| ATOM | 657 | CG  | HIS | A | 98  | 7.936  | 32.942 | 33.309 | 1.00 | 28.53 | C |
| ATOM | 658 | ND1 | HIS | A | 98  | 7.271  | 33.944 | 33.984 | 1.00 | 29.18 | N |
| ATOM | 659 | CD2 | HIS | A | 98  | 8.793  | 33.566 | 32.463 | 1.00 | 29.68 | C |
| ATOM | 660 | CE1 | HIS | A | 98  | 7.708  | 35.120 | 33.568 | 1.00 | 29.42 | C |
| ATOM | 661 | NE2 | HIS | A | 98  | 8.638  | 34.919 | 32.650 | 1.00 | 29.10 | N |
| ATOM | 662 | N   | LYS | A | 99  | 10.562 | 31.874 | 35.299 | 1.00 | 27.85 | N |
| ATOM | 663 | CA  | LYS | A | 99  | 11.997 | 32.041 | 35.124 | 1.00 | 28.24 | C |
| ATOM | 664 | C   | LYS | A | 99  | 12.878 | 31.143 | 35.997 | 1.00 | 27.69 | C |
| ATOM | 665 | O   | LYS | A | 99  | 12.892 | 31.278 | 37.216 | 1.00 | 29.10 | O |
| ATOM | 666 | CB  | LYS | A | 99  | 12.366 | 33.498 | 35.349 | 1.00 | 28.47 | C |
| ATOM | 667 | CG  | LYS | A | 99  | 11.836 | 34.410 | 34.255 | 1.00 | 30.42 | C |
| ATOM | 668 | CD  | LYS | A | 99  | 12.431 | 35.791 | 34.347 | 1.00 | 32.66 | C |
| ATOM | 669 | CE  | LYS | A | 99  | 11.757 | 36.624 | 35.421 | 1.00 | 34.45 | C |
| ATOM | 670 | NZ  | LYS | A | 99  | 10.569 | 37.347 | 34.884 | 1.00 | 35.39 | N |
| ATOM | 671 | N   | PHE | A | 100 | 13.621 | 30.237 | 35.376 | 1.00 | 26.40 | N |
| ATOM | 672 | CA  | PHE | A | 100 | 14.551 | 29.397 | 36.127 | 1.00 | 25.95 | C |
| ATOM | 673 | C   | PHE | A | 100 | 15.978 | 29.920 | 35.995 | 1.00 | 25.87 | C |
| ATOM | 674 | O   | PHE | A | 100 | 16.809 | 29.386 | 35.247 | 1.00 | 25.86 | O |
| ATOM | 675 | CB  | PHE | A | 100 | 14.469 | 27.945 | 35.686 | 1.00 | 25.48 | C |
| ATOM | 676 | CG  | PHE | A | 100 | 13.211 | 27.267 | 36.109 | 1.00 | 25.06 | C |
| ATOM | 677 | CD1 | PHE | A | 100 | 12.047 | 27.436 | 35.388 | 1.00 | 24.80 | C |
| ATOM | 678 | CD2 | PHE | A | 100 | 13.191 | 26.472 | 37.238 | 1.00 | 25.18 | C |
| ATOM | 679 | CE1 | PHE | A | 100 | 10.886 | 26.805 | 35.772 | 1.00 | 25.96 | C |
| ATOM | 680 | CE2 | PHE | A | 100 | 12.030 | 25.835 | 37.631 | 1.00 | 25.79 | C |
| ATOM | 681 | CZ  | PHE | A | 100 | 10.878 | 26.004 | 36.898 | 1.00 | 26.05 | C |
| ATOM | 682 | N   | LEU | A | 101 | 16.237 | 30.997 | 36.709 | 1.00 | 25.77 | N |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 683 | CA  | LEU | A | 101 | 17.549 | 31.589 | 36.747 | 1.00 | 25.85 | C |
| ATOM | 684 | C   | LEU | A | 101 | 18.527 | 30.605 | 37.381 | 1.00 | 25.87 | C |
| ATOM | 685 | O   | LEU | A | 101 | 18.319 | 30.136 | 38.503 | 1.00 | 24.99 | O |
| ATOM | 686 | CB  | LEU | A | 101 | 17.488 | 32.876 | 37.559 | 1.00 | 25.84 | C |
| ATOM | 687 | CG  | LEU | A | 101 | 18.795 | 33.656 | 37.708 | 1.00 | 26.07 | C |
| ATOM | 688 | CD1 | LEU | A | 101 | 19.244 | 34.200 | 36.377 | 1.00 | 25.11 | C |
| ATOM | 689 | CD2 | LEU | A | 101 | 18.609 | 34.800 | 38.710 | 1.00 | 27.75 | C |
| ATOM | 690 | N   | TYR | A | 102 | 19.582 | 30.274 | 36.644 | 1.00 | 26.56 | N |
| ATOM | 691 | CA  | TYR | A | 102 | 20.611 | 29.380 | 37.159 | 1.00 | 26.99 | C |
| ATOM | 692 | C   | TYR | A | 102 | 21.430 | 30.072 | 38.260 | 1.00 | 27.10 | C |
| ATOM | 693 | O   | TYR | A | 102 | 21.711 | 31.264 | 38.174 | 1.00 | 27.00 | O |
| ATOM | 694 | CB  | TYR | A | 102 | 21.562 | 28.939 | 36.053 | 1.00 | 27.26 | C |
| ATOM | 695 | CG  | TYR | A | 102 | 22.667 | 28.088 | 36.620 | 1.00 | 28.93 | C |
| ATOM | 696 | CD1 | TYR | A | 102 | 22.457 | 26.750 | 36.914 | 1.00 | 29.52 | C |
| ATOM | 697 | CD2 | TYR | A | 102 | 23.906 | 28.636 | 36.909 | 1.00 | 31.11 | C |
| ATOM | 698 | CE1 | TYR | A | 102 | 23.463 | 25.979 | 37.480 | 1.00 | 32.23 | C |
| ATOM | 699 | CE2 | TYR | A | 102 | 24.913 | 27.872 | 37.470 | 1.00 | 32.52 | C |
| ATOM | 700 | CZ  | TYR | A | 102 | 24.693 | 26.549 | 37.750 | 1.00 | 33.88 | C |
| ATOM | 701 | OH  | TYR | A | 102 | 25.727 | 25.794 | 38.314 | 1.00 | 38.68 | O |
| ATOM | 702 | N   | TYR | A | 103 | 21.793 | 29.322 | 39.296 | 1.00 | 26.83 | N |
| ATOM | 703 | CA  | TYR | A | 103 | 22.667 | 29.840 | 40.343 | 1.00 | 27.22 | C |
| ATOM | 704 | C   | TYR | A | 103 | 23.613 | 28.750 | 40.834 | 1.00 | 26.77 | C |
| ATOM | 705 | O   | TYR | A | 103 | 23.287 | 27.556 | 40.853 | 1.00 | 25.60 | O |
| ATOM | 706 | CB  | TYR | A | 103 | 21.880 | 30.440 | 41.517 | 1.00 | 27.38 | C |
| ATOM | 707 | CG  | TYR | A | 103 | 20.909 | 29.493 | 42.154 | 1.00 | 29.11 | C |
| ATOM | 708 | CD1 | TYR | A | 103 | 19.639 | 29.340 | 41.639 | 1.00 | 30.58 | C |
| ATOM | 709 | CD2 | TYR | A | 103 | 21.257 | 28.759 | 43.279 | 1.00 | 32.13 | C |
| ATOM | 710 | CE1 | TYR | A | 103 | 18.734 | 28.469 | 42.212 | 1.00 | 32.78 | C |
| ATOM | 711 | CE2 | TYR | A | 103 | 20.357 | 27.887 | 43.877 | 1.00 | 33.15 | C |
| ATOM | 712 | CZ  | TYR | A | 103 | 19.096 | 27.745 | 43.329 | 1.00 | 34.41 | C |
| ATOM | 713 | OH  | TYR | A | 103 | 18.187 | 26.888 | 43.892 | 1.00 | 37.44 | O |
| ATOM | 714 | N   | ASP | A | 104 | 24.798 | 29.182 | 41.225 | 1.00 | 26.36 | N |
| ATOM | 715 | CA  | ASP | A | 104 | 25.832 | 28.273 | 41.673 | 1.00 | 26.28 | C |
| ATOM | 716 | C   | ASP | A | 104 | 25.802 | 28.239 | 43.184 | 1.00 | 26.21 | C |
| ATOM | 717 | O   | ASP | A | 104 | 26.163 | 29.212 | 43.845 | 1.00 | 25.45 | O |
| ATOM | 718 | CB  | ASP | A | 104 | 27.174 | 28.765 | 41.154 | 1.00 | 25.92 | C |
| ATOM | 719 | CG  | ASP | A | 104 | 28.330 | 27.889 | 41.575 | 1.00 | 27.39 | C |
| ATOM | 720 | OD1 | ASP | A | 104 | 28.161 | 26.973 | 42.437 | 1.00 | 27.13 | O |
| ATOM | 721 | OD2 | ASP | A | 104 | 29.459 | 28.068 | 41.075 | 1.00 | 27.68 | O |
| ATOM | 722 | N   | GLU | A | 105 | 25.358 | 27.114 | 43.724 | 1.00 | 26.46 | N |
| ATOM | 723 | CA  | GLU | A | 105 | 25.218 | 26.962 | 45.162 | 1.00 | 27.02 | C |
| ATOM | 724 | C   | GLU | A | 105 | 26.540 | 27.199 | 45.916 | 1.00 | 26.91 | C |
| ATOM | 725 | O   | GLU | A | 105 | 26.523 | 27.718 | 47.026 | 1.00 | 26.51 | O |
| ATOM | 726 | CB  | GLU | A | 105 | 24.602 | 25.587 | 45.481 | 1.00 | 27.45 | C |
| ATOM | 727 | CG  | GLU | A | 105 | 23.088 | 25.556 | 45.254 | 1.00 | 29.46 | C |
| ATOM | 728 | CD  | GLU | A | 105 | 22.527 | 24.158 | 45.025 | 1.00 | 32.85 | C |
| ATOM | 729 | OE1 | GLU | A | 105 | 22.908 | 23.234 | 45.765 | 1.00 | 32.90 | O |
| ATOM | 730 | OE2 | GLU | A | 105 | 21.703 | 23.980 | 44.085 | 1.00 | 35.16 | O |
| ATOM | 731 | N   | LYS | A | 106 | 27.680 | 26.874 | 45.305 | 1.00 | 27.12 | N |
| ATOM | 732 | CA  | LYS | A | 106 | 28.979 | 27.041 | 45.983 | 1.00 | 27.54 | C |
| ATOM | 733 | C   | LYS | A | 106 | 29.331 | 28.493 | 46.258 | 1.00 | 27.70 | C |
| ATOM | 734 | O   | LYS | A | 106 | 30.164 | 28.769 | 47.099 | 1.00 | 27.61 | O |
| ATOM | 735 | CB  | LYS | A | 106 | 30.127 | 26.441 | 45.163 | 1.00 | 27.58 | C |
| ATOM | 736 | CG  | LYS | A | 106 | 30.038 | 24.928 | 44.918 | 1.00 | 28.61 | C |
| ATOM | 737 | N   | LYS | A | 107 | 28.713 | 29.420 | 45.537 | 1.00 | 27.99 | N |
| ATOM | 738 | CA  | LYS | A | 107 | 29.020 | 30.826 | 45.694 | 1.00 | 28.30 | C |
| ATOM | 739 | C   | LYS | A | 107 | 28.034 | 31.513 | 46.631 | 1.00 | 29.21 | C |
| ATOM | 740 | O   | LYS | A | 107 | 28.175 | 32.701 | 46.917 | 1.00 | 29.08 | O |
| ATOM | 741 | CB  | LYS | A | 107 | 29.040 | 31.524 | 44.324 | 1.00 | 28.30 | C |
| ATOM | 742 | CG  | LYS | A | 107 | 30.344 | 31.291 | 43.516 | 1.00 | 28.07 | C |
| ATOM | 743 | CD  | LYS | A | 107 | 30.242 | 31.737 | 42.034 | 1.00 | 27.29 | C |



|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 744 | CE  | LYS | A | 107 | 31.584 | 31.518 | 41.315 | 1.00 | 26.86 | C |
| ATOM | 745 | NZ  | LYS | A | 107 | 31.642 | 31.889 | 39.870 | 1.00 | 24.80 | N |
| ATOM | 746 | N   | MET | A | 108 | 27.041 | 30.781 | 47.125 | 1.00 | 30.08 | N |
| ATOM | 747 | CA  | MET | A | 108 | 26.031 | 31.405 | 47.982 | 1.00 | 31.53 | C |
| ATOM | 748 | C   | MET | A | 108 | 26.581 | 31.952 | 49.309 | 1.00 | 32.44 | C |
| ATOM | 749 | O   | MET | A | 108 | 26.102 | 32.972 | 49.812 | 1.00 | 32.47 | O |
| ATOM | 750 | CB  | MET | A | 108 | 24.862 | 30.452 | 48.218 | 1.00 | 31.81 | C |
| ATOM | 751 | CG  | MET | A | 108 | 24.072 | 30.193 | 46.932 | 1.00 | 33.07 | C |
| ATOM | 752 | SD  | MET | A | 108 | 22.625 | 29.140 | 47.064 | 1.00 | 35.76 | S |
| ATOM | 753 | CE  | MET | A | 108 | 21.540 | 30.140 | 48.050 | 1.00 | 35.99 | C |
| ATOM | 754 | N   | ALA | A | 109 | 27.603 | 31.315 | 49.860 | 1.00 | 33.56 | N |
| ATOM | 755 | CA  | ALA | A | 109 | 28.154 | 31.769 | 51.138 | 1.00 | 34.94 | C |
| ATOM | 756 | C   | ALA | A | 109 | 28.651 | 33.212 | 51.060 | 1.00 | 35.81 | C |
| ATOM | 757 | O   | ALA | A | 109 | 28.483 | 33.989 | 51.991 | 1.00 | 36.23 | O |
| ATOM | 758 | CB  | ALA | A | 109 | 29.279 | 30.838 | 51.606 | 1.00 | 34.82 | C |
| ATOM | 759 | N   | ASN | A | 110 | 29.236 | 33.575 | 49.929 | 1.00 | 37.05 | N |
| ATOM | 760 | CA  | ASN | A | 110 | 29.774 | 34.918 | 49.748 | 1.00 | 37.94 | C |
| ATOM | 761 | C   | ASN | A | 110 | 28.731 | 35.992 | 49.413 | 1.00 | 38.13 | C |
| ATOM | 762 | O   | ASN | A | 110 | 29.064 | 37.167 | 49.293 | 1.00 | 37.92 | O |
| ATOM | 763 | CB  | ASN | A | 110 | 30.855 | 34.878 | 48.669 | 1.00 | 38.16 | C |
| ATOM | 764 | CG  | ASN | A | 110 | 32.050 | 34.035 | 49.079 | 1.00 | 39.37 | C |
| ATOM | 765 | OD1 | ASN | A | 110 | 32.407 | 33.964 | 50.265 | 1.00 | 40.12 | O |
| ATOM | 766 | ND2 | ASN | A | 110 | 32.670 | 33.377 | 48.103 | 1.00 | 39.46 | N |
| ATOM | 767 | N   | PHE | A | 111 | 27.480 | 35.588 | 49.234 | 1.00 | 38.71 | N |
| ATOM | 768 | CA  | PHE | A | 111 | 26.408 | 36.539 | 48.966 | 1.00 | 39.02 | C |
| ATOM | 769 | C   | PHE | A | 111 | 25.180 | 36.135 | 49.773 | 1.00 | 39.71 | C |
| ATOM | 770 | O   | PHE | A | 111 | 24.143 | 35.747 | 49.232 | 1.00 | 39.45 | O |
| ATOM | 771 | CB  | PHE | A | 111 | 26.091 | 36.603 | 47.471 | 1.00 | 38.97 | C |
| ATOM | 772 | CG  | PHE | A | 111 | 27.110 | 37.362 | 46.672 | 1.00 | 38.04 | C |
| ATOM | 773 | CD1 | PHE | A | 111 | 28.329 | 36.791 | 46.363 | 1.00 | 37.99 | C |
| ATOM | 774 | CD2 | PHE | A | 111 | 26.851 | 38.642 | 46.235 | 1.00 | 36.83 | C |
| ATOM | 775 | CE1 | PHE | A | 111 | 29.269 | 37.493 | 45.635 | 1.00 | 37.68 | C |
| ATOM | 776 | CE2 | PHE | A | 111 | 27.788 | 39.339 | 45.500 | 1.00 | 36.08 | C |
| ATOM | 777 | CZ  | PHE | A | 111 | 28.994 | 38.768 | 45.208 | 1.00 | 35.84 | C |
| ATOM | 778 | N   | GLN | A | 112 | 25.315 | 36.267 | 51.085 | 1.00 | 40.62 | N |
| ATOM | 779 | CA  | GLN | A | 112 | 24.286 | 35.852 | 52.029 | 1.00 | 41.31 | C |
| ATOM | 780 | C   | GLN | A | 112 | 22.915 | 36.430 | 51.721 | 1.00 | 41.10 | C |
| ATOM | 781 | O   | GLN | A | 112 | 21.906 | 35.827 | 52.060 | 1.00 | 41.31 | O |
| ATOM | 782 | CB  | GLN | A | 112 | 24.701 | 36.236 | 53.451 | 1.00 | 41.65 | C |
| ATOM | 783 | CG  | GLN | A | 112 | 26.058 | 35.694 | 53.882 | 1.00 | 43.80 | C |
| ATOM | 784 | CD  | GLN | A | 112 | 26.104 | 34.177 | 53.938 | 1.00 | 46.42 | C |
| ATOM | 785 | OE1 | GLN | A | 112 | 25.394 | 33.501 | 53.191 | 1.00 | 48.56 | O |
| ATOM | 786 | NE2 | GLN | A | 112 | 26.951 | 33.637 | 54.816 | 1.00 | 46.94 | N |
| ATOM | 787 | N   | ASN | A | 113 | 22.876 | 37.588 | 51.074 | 1.00 | 41.02 | N |
| ATOM | 788 | CA  | ASN | A | 113 | 21.606 | 38.229 | 50.749 | 1.00 | 40.98 | C |
| ATOM | 789 | C   | ASN | A | 113 | 20.954 | 37.760 | 49.440 | 1.00 | 40.71 | C |
| ATOM | 790 | O   | ASN | A | 113 | 19.889 | 38.251 | 49.071 | 1.00 | 40.77 | O |
| ATOM | 791 | CB  | ASN | A | 113 | 21.778 | 39.753 | 50.737 | 1.00 | 41.09 | C |
| ATOM | 792 | CG  | ASN | A | 113 | 22.129 | 40.314 | 52.123 | 1.00 | 41.51 | C |
| ATOM | 793 | OD1 | ASN | A | 113 | 21.717 | 39.772 | 53.158 | 1.00 | 40.60 | O |
| ATOM | 794 | ND2 | ASN | A | 113 | 22.892 | 41.401 | 52.141 | 1.00 | 41.19 | N |
| ATOM | 795 | N   | PHE | A | 114 | 21.571 | 36.826 | 48.725 | 1.00 | 40.34 | N |
| ATOM | 796 | CA  | PHE | A | 114 | 20.934 | 36.321 | 47.515 | 1.00 | 39.86 | C |
| ATOM | 797 | C   | PHE | A | 114 | 19.908 | 35.266 | 47.902 | 1.00 | 39.46 | C |
| ATOM | 798 | O   | PHE | A | 114 | 20.235 | 34.299 | 48.584 | 1.00 | 38.82 | O |
| ATOM | 799 | CB  | PHE | A | 114 | 21.940 | 35.714 | 46.552 | 1.00 | 39.96 | C |
| ATOM | 800 | CG  | PHE | A | 114 | 21.298 | 35.059 | 45.362 | 1.00 | 40.54 | C |
| ATOM | 801 | CD1 | PHE | A | 114 | 20.670 | 35.828 | 44.395 | 1.00 | 40.29 | C |
| ATOM | 802 | CD2 | PHE | A | 114 | 21.295 | 33.679 | 45.224 | 1.00 | 40.62 | C |
| ATOM | 803 | CE1 | PHE | A | 114 | 20.061 | 35.237 | 43.307 | 1.00 | 40.20 | C |
| ATOM | 804 | CE2 | PHE | A | 114 | 20.684 | 33.082 | 44.126 | 1.00 | 40.36 | C |



|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 805 | CZ  | PHE | A | 114 | 20.066 | 33.866 | 43.172 | 1.00 | 40.52 | C |
| ATOM | 806 | N   | LYS | A | 115 | 18.669 | 35.457 | 47.461 | 1.00 | 39.11 | N |
| ATOM | 807 | CA  | LYS | A | 115 | 17.596 | 34.529 | 47.787 | 1.00 | 39.02 | C |
| ATOM | 808 | C   | LYS | A | 115 | 17.042 | 33.938 | 46.497 | 1.00 | 38.71 | C |
| ATOM | 809 | O   | LYS | A | 115 | 16.285 | 34.590 | 45.787 | 1.00 | 39.00 | O |
| ATOM | 810 | CB  | LYS | A | 115 | 16.498 | 35.251 | 48.578 | 1.00 | 39.14 | C |
| ATOM | 811 | N   | PRO | A | 116 | 17.389 | 32.691 | 46.213 | 1.00 | 38.17 | N |
| ATOM | 812 | CA  | PRO | A | 116 | 17.027 | 32.060 | 44.938 | 1.00 | 37.95 | C |
| ATOM | 813 | C   | PRO | A | 116 | 15.532 | 31.889 | 44.783 | 1.00 | 37.38 | C |
| ATOM | 814 | O   | PRO | A | 116 | 14.865 | 31.506 | 45.733 | 1.00 | 37.36 | O |
| ATOM | 815 | CB  | PRO | A | 116 | 17.684 | 30.679 | 45.004 | 1.00 | 38.15 | C |
| ATOM | 816 | CG  | PRO | A | 116 | 18.416 | 30.604 | 46.297 | 1.00 | 38.40 | C |
| ATOM | 817 | CD  | PRO | A | 116 | 18.079 | 31.775 | 47.125 | 1.00 | 38.19 | C |
| ATOM | 818 | N   | ARG | A | 117 | 15.027 | 32.161 | 43.590 | 1.00 | 36.84 | N |
| ATOM | 819 | CA  | ARG | A | 117 | 13.611 | 32.028 | 43.293 | 1.00 | 36.61 | C |
| ATOM | 820 | C   | ARG | A | 117 | 13.259 | 30.581 | 42.984 | 1.00 | 36.38 | C |
| ATOM | 821 | O   | ARG | A | 117 | 12.084 | 30.230 | 42.913 | 1.00 | 36.44 | O |
| ATOM | 822 | CB  | ARG | A | 117 | 13.235 | 32.913 | 42.122 | 1.00 | 36.62 | C |
| ATOM | 823 | N   | SER | A | 118 | 14.271 | 29.745 | 42.777 | 1.00 | 35.79 | N |
| ATOM | 824 | CA  | SER | A | 118 | 14.025 | 28.339 | 42.538 | 1.00 | 35.51 | C |
| ATOM | 825 | C   | SER | A | 118 | 14.844 | 27.491 | 43.512 | 1.00 | 35.35 | C |
| ATOM | 826 | O   | SER | A | 118 | 15.888 | 27.923 | 43.991 | 1.00 | 35.16 | O |
| ATOM | 827 | CB  | SER | A | 118 | 14.330 | 27.976 | 41.086 | 1.00 | 35.26 | C |
| ATOM | 828 | OG  | SER | A | 118 | 15.689 | 28.164 | 40.795 | 1.00 | 35.14 | O |
| ATOM | 829 | N   | ASN | A | 119 | 14.329 | 26.306 | 43.824 | 1.00 | 35.11 | N |
| ATOM | 830 | CA  | ASN | A | 119 | 14.997 | 25.373 | 44.715 | 1.00 | 35.21 | C |
| ATOM | 831 | C   | ASN | A | 119 | 15.233 | 24.049 | 44.022 | 1.00 | 34.26 | C |
| ATOM | 832 | O   | ASN | A | 119 | 14.401 | 23.595 | 43.244 | 1.00 | 34.11 | O |
| ATOM | 833 | CB  | ASN | A | 119 | 14.145 | 25.110 | 45.957 | 1.00 | 35.95 | C |
| ATOM | 834 | CG  | ASN | A | 119 | 13.636 | 26.382 | 46.592 | 1.00 | 38.47 | C |
| ATOM | 835 | OD1 | ASN | A | 119 | 14.417 | 27.245 | 47.025 | 1.00 | 41.76 | O |
| ATOM | 836 | ND2 | ASN | A | 119 | 12.314 | 26.511 | 46.657 | 1.00 | 42.21 | N |
| ATOM | 837 | N   | ARG | A | 120 | 16.368 | 23.434 | 44.326 | 1.00 | 33.75 | N |
| ATOM | 838 | CA  | ARG | A | 120 | 16.750 | 22.149 | 43.761 | 1.00 | 33.33 | C |
| ATOM | 839 | C   | ARG | A | 120 | 16.327 | 21.045 | 44.699 | 1.00 | 33.26 | C |
| ATOM | 840 | O   | ARG | A | 120 | 16.523 | 21.138 | 45.910 | 1.00 | 33.07 | O |
| ATOM | 841 | CB  | ARG | A | 120 | 18.270 | 22.075 | 43.592 | 1.00 | 33.37 | C |
| ATOM | 842 | CG  | ARG | A | 120 | 18.759 | 20.889 | 42.771 | 1.00 | 32.70 | C |
| ATOM | 843 | CD  | ARG | A | 120 | 20.277 | 20.732 | 42.743 | 1.00 | 31.64 | C |
| ATOM | 844 | NE  | ARG | A | 120 | 20.892 | 21.165 | 43.992 | 1.00 | 31.16 | N |
| ATOM | 845 | CZ  | ARG | A | 120 | 21.233 | 20.357 | 44.993 | 1.00 | 31.33 | C |
| ATOM | 846 | NH1 | ARG | A | 120 | 21.027 | 19.047 | 44.920 | 1.00 | 30.77 | N |
| ATOM | 847 | NH2 | ARG | A | 120 | 21.789 | 20.867 | 46.077 | 1.00 | 31.01 | N |
| ATOM | 848 | N   | GLU | A | 121 | 15.735 | 20.001 | 44.137 | 1.00 | 32.98 | N |
| ATOM | 849 | CA  | GLU | A | 121 | 15.379 | 18.827 | 44.904 | 1.00 | 32.85 | C |
| ATOM | 850 | C   | GLU | A | 121 | 15.846 | 17.630 | 44.095 | 1.00 | 32.17 | C |
| ATOM | 851 | O   | GLU | A | 121 | 15.744 | 17.612 | 42.864 | 1.00 | 32.36 | O |
| ATOM | 852 | CB  | GLU | A | 121 | 13.874 | 18.767 | 45.179 | 1.00 | 33.21 | C |
| ATOM | 853 | CG  | GLU | A | 121 | 13.420 | 17.468 | 45.826 | 1.00 | 35.39 | C |
| ATOM | 854 | CD  | GLU | A | 121 | 12.189 | 17.629 | 46.699 | 1.00 | 38.11 | C |
| ATOM | 855 | OE1 | GLU | A | 121 | 12.326 | 18.152 | 47.830 | 1.00 | 41.26 | O |
| ATOM | 856 | OE2 | GLU | A | 121 | 11.091 | 17.221 | 46.270 | 1.00 | 39.55 | O |
| ATOM | 857 | N   | GLU | A | 122 | 16.400 | 16.648 | 44.786 | 1.00 | 31.28 | N |
| ATOM | 858 | CA  | GLU | A | 122 | 16.886 | 15.448 | 44.150 | 1.00 | 30.61 | C |
| ATOM | 859 | C   | GLU | A | 122 | 15.814 | 14.392 | 44.298 | 1.00 | 30.31 | C |
| ATOM | 860 | O   | GLU | A | 122 | 15.328 | 14.165 | 45.395 | 1.00 | 30.07 | O |
| ATOM | 861 | CB  | GLU | A | 122 | 18.163 | 14.980 | 44.833 | 1.00 | 30.52 | C |
| ATOM | 862 | CG  | GLU | A | 122 | 19.293 | 15.983 | 44.771 | 1.00 | 29.67 | C |
| ATOM | 863 | CD  | GLU | A | 122 | 19.747 | 16.253 | 43.348 | 1.00 | 29.79 | C |
| ATOM | 864 | OE1 | GLU | A | 122 | 20.120 | 15.280 | 42.667 | 1.00 | 28.28 | O |
| ATOM | 865 | OE2 | GLU | A | 122 | 19.734 | 17.439 | 42.914 | 1.00 | 27.93 | O |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 866 | N   | MET | A | 123 | 15.432 | 13.751 | 43.202 | 1.00 | 29.74 | N |
| ATOM | 867 | CA  | MET | A | 123 | 14.407 | 12.728 | 43.277 | 1.00 | 29.77 | C |
| ATOM | 868 | C   | MET | A | 123 | 14.594 | 11.683 | 42.202 | 1.00 | 29.31 | C |
| ATOM | 869 | O   | MET | A | 123 | 15.408 | 11.842 | 41.294 | 1.00 | 29.42 | O |
| ATOM | 870 | CB  | MET | A | 123 | 13.016 | 13.354 | 43.165 | 1.00 | 29.81 | C |
| ATOM | 871 | CG  | MET | A | 123 | 12.749 | 14.057 | 41.865 | 1.00 | 30.27 | C |
| ATOM | 872 | SD  | MET | A | 123 | 11.181 | 14.960 | 41.871 | 1.00 | 31.65 | S |
| ATOM | 873 | CE  | MET | A | 123 | 11.582 | 16.371 | 42.804 | 1.00 | 31.47 | C |
| ATOM | 874 | N   | LYS | A | 124 | 13.835 | 10.604 | 42.332 | 1.00 | 28.82 | N |
| ATOM | 875 | CA  | LYS | A | 124 | 13.841 | 9.535  | 41.352 | 1.00 | 28.33 | C |
| ATOM | 876 | C   | LYS | A | 124 | 12.959 | 9.976  | 40.191 | 1.00 | 27.51 | C |
| ATOM | 877 | O   | LYS | A | 124 | 12.077 | 10.817 | 40.361 | 1.00 | 26.52 | O |
| ATOM | 878 | CB  | LYS | A | 124 | 13.330 | 8.242  | 41.984 | 1.00 | 28.45 | C |
| ATOM | 879 | CG  | LYS | A | 124 | 14.153 | 7.783  | 43.204 | 1.00 | 29.42 | C |
| ATOM | 880 | CD  | LYS | A | 124 | 15.597 | 7.442  | 42.804 | 1.00 | 30.46 | C |
| ATOM | 881 | CE  | LYS | A | 124 | 16.479 | 7.067  | 43.992 | 1.00 | 30.52 | C |
| ATOM | 882 | NZ  | LYS | A | 124 | 17.928 | 7.324  | 43.699 | 1.00 | 30.05 | N |
| ATOM | 883 | N   | PHE | A | 125 | 13.188 | 9.407  | 39.014 | 1.00 | 26.98 | N |
| ATOM | 884 | CA  | PHE | A | 125 | 12.477 | 9.871  | 37.826 | 1.00 | 26.83 | C |
| ATOM | 885 | C   | PHE | A | 125 | 10.974 | 9.762  | 37.972 | 1.00 | 26.77 | C |
| ATOM | 886 | O   | PHE | A | 125 | 10.245 | 10.673 | 37.585 | 1.00 | 26.38 | O |
| ATOM | 887 | CB  | PHE | A | 125 | 12.927 | 9.138  | 36.568 | 1.00 | 26.71 | C |
| ATOM | 888 | CG  | PHE | A | 125 | 12.613 | 9.891  | 35.316 | 1.00 | 26.32 | C |
| ATOM | 889 | CD1 | PHE | A | 125 | 13.476 | 10.876 | 34.849 | 1.00 | 26.29 | C |
| ATOM | 890 | CD2 | PHE | A | 125 | 11.438 | 9.657  | 34.635 | 1.00 | 26.06 | C |
| ATOM | 891 | CE1 | PHE | A | 125 | 13.183 | 11.594 | 33.715 | 1.00 | 25.70 | C |
| ATOM | 892 | CE2 | PHE | A | 125 | 11.140 | 10.368 | 33.483 | 1.00 | 26.70 | C |
| ATOM | 893 | CZ  | PHE | A | 125 | 12.018 | 11.341 | 33.025 | 1.00 | 26.87 | C |
| ATOM | 894 | N   | HIS | A | 126 | 10.527 | 8.649  | 38.550 | 1.00 | 26.77 | N |
| ATOM | 895 | CA  | HIS | A | 126 | 9.113  | 8.396  | 38.753 | 1.00 | 26.82 | C |
| ATOM | 896 | C   | HIS | A | 126 | 8.517  | 9.390  | 39.734 | 1.00 | 26.68 | C |
| ATOM | 897 | O   | HIS | A | 126 | 7.326  | 9.670  | 39.687 | 1.00 | 26.03 | O |
| ATOM | 898 | CB  | HIS | A | 126 | 8.882  | 6.951  | 39.238 | 1.00 | 27.07 | C |
| ATOM | 899 | CG  | HIS | A | 126 | 9.028  | 6.767  | 40.717 | 1.00 | 27.39 | C |
| ATOM | 900 | ND1 | HIS | A | 126 | 7.959  | 6.836  | 41.582 | 1.00 | 28.48 | N |
| ATOM | 901 | CD2 | HIS | A | 126 | 10.115 | 6.505  | 41.484 | 1.00 | 28.33 | C |
| ATOM | 902 | CE1 | HIS | A | 126 | 8.382  | 6.636  | 42.819 | 1.00 | 28.68 | C |
| ATOM | 903 | NE2 | HIS | A | 126 | 9.687  | 6.439  | 42.788 | 1.00 | 27.97 | N |
| ATOM | 904 | N   | GLU | A | 127 | 9.342  | 9.918  | 40.630 | 1.00 | 27.00 | N |
| ATOM | 905 | CA  | GLU | A | 127 | 8.876  | 10.930 | 41.572 | 1.00 | 27.34 | C |
| ATOM | 906 | C   | GLU | A | 127 | 8.683  | 12.259 | 40.838 | 1.00 | 27.36 | C |
| ATOM | 907 | O   | GLU | A | 127 | 7.761  | 13.026 | 41.126 | 1.00 | 26.86 | O |
| ATOM | 908 | CB  | GLU | A | 127 | 9.862  | 11.084 | 42.728 | 1.00 | 27.31 | C |
| ATOM | 909 | CG  | GLU | A | 127 | 10.018 | 9.821  | 43.552 | 1.00 | 28.69 | C |
| ATOM | 910 | CD  | GLU | A | 127 | 10.959 | 9.992  | 44.722 | 1.00 | 29.65 | C |
| ATOM | 911 | OE1 | GLU | A | 127 | 12.139 | 10.318 | 44.485 | 1.00 | 29.56 | O |
| ATOM | 912 | OE2 | GLU | A | 127 | 10.509 | 9.787  | 45.876 | 1.00 | 30.92 | O |
| ATOM | 913 | N   | PHE | A | 128 | 9.554  | 12.519 | 39.876 | 1.00 | 27.91 | N |
| ATOM | 914 | CA  | PHE | A | 128 | 9.453  | 13.736 | 39.068 | 1.00 | 28.21 | C |
| ATOM | 915 | C   | PHE | A | 128 | 8.149  | 13.658 | 38.282 | 1.00 | 29.04 | C |
| ATOM | 916 | O   | PHE | A | 128 | 7.354  | 14.600 | 38.255 | 1.00 | 29.03 | O |
| ATOM | 917 | CB  | PHE | A | 128 | 10.643 | 13.838 | 38.115 | 1.00 | 27.74 | C |
| ATOM | 918 | CG  | PHE | A | 128 | 10.427 | 14.792 | 36.959 | 1.00 | 27.06 | C |
| ATOM | 919 | CD1 | PHE | A | 128 | 10.189 | 16.138 | 37.185 | 1.00 | 25.41 | C |
| ATOM | 920 | CD2 | PHE | A | 128 | 10.480 | 14.343 | 35.657 | 1.00 | 25.60 | C |
| ATOM | 921 | CE1 | PHE | A | 128 | 9.985  | 17.000 | 36.144 | 1.00 | 25.41 | C |
| ATOM | 922 | CE2 | PHE | A | 128 | 10.281 | 15.215 | 34.604 | 1.00 | 26.59 | C |
| ATOM | 923 | CZ  | PHE | A | 128 | 10.032 | 16.540 | 34.846 | 1.00 | 25.61 | C |
| ATOM | 924 | N   | VAL | A | 129 | 7.925  | 12.500 | 37.677 | 1.00 | 29.90 | N |
| ATOM | 925 | CA  | VAL | A | 129 | 6.756  | 12.285 | 36.847 | 1.00 | 30.82 | C |
| ATOM | 926 | C   | VAL | A | 129 | 5.476  | 12.447 | 37.669 | 1.00 | 31.61 | C |

|      |     |     |           |        |        |        |      |       |   |
|------|-----|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 927 | O   | VAL A 129 | 4.515  | 13.091 | 37.234 | 1.00 | 31.39 | O |
| ATOM | 928 | CB  | VAL A 129 | 6.793  | 10.883 | 36.213 | 1.00 | 30.92 | C |
| ATOM | 929 | CG1 | VAL A 129 | 5.479  | 10.582 | 35.503 | 1.00 | 31.15 | C |
| ATOM | 930 | CG2 | VAL A 129 | 7.975  | 10.751 | 35.253 | 1.00 | 30.61 | C |
| ATOM | 931 | N   | GLU A 130 | 5.475  | 11.858 | 38.861 | 1.00 | 32.42 | N |
| ATOM | 932 | CA  | GLU A 130 | 4.332  | 11.946 | 39.761 | 1.00 | 33.13 | C |
| ATOM | 933 | C   | GLU A 130 | 4.070  | 13.403 | 40.126 | 1.00 | 33.42 | C |
| ATOM | 934 | O   | GLU A 130 | 2.930  | 13.867 | 40.081 | 1.00 | 33.01 | O |
| ATOM | 935 | CB  | GLU A 130 | 4.587  | 11.108 | 41.017 | 1.00 | 33.20 | C |
| ATOM | 936 | CG  | GLU A 130 | 4.537  | 9.609  | 40.755 | 1.00 | 34.22 | C |
| ATOM | 937 | CD  | GLU A 130 | 5.294  | 8.792  | 41.789 | 1.00 | 35.55 | C |
| ATOM | 938 | OE1 | GLU A 130 | 5.630  | 9.339  | 42.861 | 1.00 | 37.02 | O |
| ATOM | 939 | OE2 | GLU A 130 | 5.558  | 7.598  | 41.525 | 1.00 | 35.99 | O |
| ATOM | 940 | N   | LYS A 131 | 5.128  | 14.120 | 40.486 | 1.00 | 34.00 | N |
| ATOM | 941 | CA  | LYS A 131 | 4.994  | 15.538 | 40.800 | 1.00 | 34.79 | C |
| ATOM | 942 | C   | LYS A 131 | 4.354  | 16.286 | 39.637 | 1.00 | 35.25 | C |
| ATOM | 943 | O   | LYS A 131 | 3.449  | 17.089 | 39.835 | 1.00 | 34.81 | O |
| ATOM | 944 | CB  | LYS A 131 | 6.345  | 16.171 | 41.100 | 1.00 | 34.89 | C |
| ATOM | 945 | CG  | LYS A 131 | 6.597  | 16.477 | 42.554 | 1.00 | 35.57 | C |
| ATOM | 946 | CD  | LYS A 131 | 7.191  | 17.868 | 42.694 | 1.00 | 36.25 | C |
| ATOM | 947 | CE  | LYS A 131 | 7.862  | 18.072 | 44.034 | 1.00 | 37.30 | C |
| ATOM | 948 | NZ  | LYS A 131 | 8.108  | 19.526 | 44.332 | 1.00 | 37.49 | N |
| ATOM | 949 | N   | LEU A 132 | 4.829  | 16.038 | 38.422 | 1.00 | 36.00 | N |
| ATOM | 950 | CA  | LEU A 132 | 4.243  | 16.701 | 37.268 | 1.00 | 37.05 | C |
| ATOM | 951 | C   | LEU A 132 | 2.755  | 16.406 | 37.170 | 1.00 | 37.67 | C |
| ATOM | 952 | O   | LEU A 132 | 1.963  | 17.300 | 36.870 | 1.00 | 37.77 | O |
| ATOM | 953 | CB  | LEU A 132 | 4.919  | 16.260 | 35.979 | 1.00 | 37.39 | C |
| ATOM | 954 | CG  | LEU A 132 | 6.310  | 16.803 | 35.710 | 1.00 | 38.29 | C |
| ATOM | 955 | CD1 | LEU A 132 | 6.783  | 16.289 | 34.363 | 1.00 | 39.35 | C |
| ATOM | 956 | CD2 | LEU A 132 | 6.306  | 18.314 | 35.721 | 1.00 | 39.70 | C |
| ATOM | 957 | N   | GLN A 133 | 2.386  | 15.151 | 37.417 | 1.00 | 38.34 | N |
| ATOM | 958 | CA  | GLN A 133 | 0.989  | 14.730 | 37.373 | 1.00 | 39.11 | C |
| ATOM | 959 | C   | GLN A 133 | 0.132  | 15.434 | 38.427 | 1.00 | 39.73 | C |
| ATOM | 960 | O   | GLN A 133 | -0.966 | 15.897 | 38.126 | 1.00 | 39.61 | O |
| ATOM | 961 | CB  | GLN A 133 | 0.886  | 13.213 | 37.538 | 1.00 | 39.05 | C |
| ATOM | 962 | N   | ASP A 134 | 0.629  | 15.507 | 39.658 | 1.00 | 40.61 | N |
| ATOM | 963 | CA  | ASP A 134 | -0.108 | 16.149 | 40.747 | 1.00 | 41.70 | C |
| ATOM | 964 | C   | ASP A 134 | -0.398 | 17.626 | 40.451 | 1.00 | 41.68 | C |
| ATOM | 965 | O   | ASP A 134 | -1.470 | 18.137 | 40.770 | 1.00 | 41.28 | O |
| ATOM | 966 | CB  | ASP A 134 | 0.678  | 16.030 | 42.056 | 1.00 | 42.32 | C |
| ATOM | 967 | CG  | ASP A 134 | -0.165 | 16.351 | 43.286 | 1.00 | 44.92 | C |
| ATOM | 968 | OD1 | ASP A 134 | -1.235 | 16.991 | 43.152 | 1.00 | 48.33 | O |
| ATOM | 969 | OD2 | ASP A 134 | 0.164  | 15.991 | 44.442 | 1.00 | 48.64 | O |
| ATOM | 970 | N   | ILE A 135 | 0.563  | 18.312 | 39.842 | 1.00 | 41.92 | N |
| ATOM | 971 | CA  | ILE A 135 | 0.383  | 19.717 | 39.512 | 1.00 | 42.18 | C |
| ATOM | 972 | C   | ILE A 135 | -0.715 | 19.862 | 38.471 | 1.00 | 42.41 | C |
| ATOM | 973 | O   | ILE A 135 | -1.635 | 20.664 | 38.634 | 1.00 | 42.49 | O |
| ATOM | 974 | CB  | ILE A 135 | 1.696  | 20.324 | 38.997 | 1.00 | 42.17 | C |
| ATOM | 975 | CG1 | ILE A 135 | 2.720  | 20.399 | 40.131 | 1.00 | 42.25 | C |
| ATOM | 976 | CG2 | ILE A 135 | 1.451  | 21.708 | 38.437 | 1.00 | 42.11 | C |
| ATOM | 977 | CD1 | ILE A 135 | 4.151  | 20.438 | 39.653 | 1.00 | 42.91 | C |
| ATOM | 978 | N   | GLN A 136 | -0.614 | 19.075 | 37.407 | 1.00 | 42.71 | N |
| ATOM | 979 | CA  | GLN A 136 | -1.593 | 19.114 | 36.333 | 1.00 | 43.09 | C |
| ATOM | 980 | C   | GLN A 136 | -2.991 | 18.935 | 36.900 | 1.00 | 43.56 | C |
| ATOM | 981 | O   | GLN A 136 | -3.863 | 19.785 | 36.707 | 1.00 | 43.93 | O |
| ATOM | 982 | CB  | GLN A 136 | -1.298 | 18.031 | 35.317 | 1.00 | 43.10 | C |
| ATOM | 983 | N   | GLN A 137 | -3.181 | 17.844 | 37.635 | 1.00 | 43.82 | N |
| ATOM | 984 | CA  | GLN A 137 | -4.486 | 17.493 | 38.182 | 1.00 | 44.02 | C |
| ATOM | 985 | C   | GLN A 137 | -5.023 | 18.540 | 39.144 | 1.00 | 44.08 | C |
| ATOM | 986 | O   | GLN A 137 | -6.202 | 18.891 | 39.080 | 1.00 | 44.46 | O |
| ATOM | 987 | CB  | GLN A 137 | -4.425 | 16.124 | 38.868 | 1.00 | 44.00 | C |



|      |      |     |           |        |        |        |      |       |   |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 988  | N   | ARG A 138 | -4.169 | 19.043 | 40.031 | 1.00 | 43.93 | N |
| ATOM | 989  | CA  | ARG A 138 | -4.606 | 20.022 | 41.024 | 1.00 | 43.76 | C |
| ATOM | 990  | C   | ARG A 138 | -4.578 | 21.445 | 40.463 | 1.00 | 43.34 | C |
| ATOM | 991  | O   | ARG A 138 | -4.681 | 22.415 | 41.214 | 1.00 | 43.54 | O |
| ATOM | 992  | CB  | ARG A 138 | -3.751 | 19.919 | 42.299 | 1.00 | 43.84 | C |
| ATOM | 993  | CG  | ARG A 138 | -2.420 | 20.679 | 42.279 | 1.00 | 44.85 | C |
| ATOM | 994  | CD  | ARG A 138 | -1.493 | 20.279 | 43.420 | 1.00 | 45.82 | C |
| ATOM | 995  | NE  | ARG A 138 | -0.372 | 21.197 | 43.620 | 1.00 | 46.44 | N |
| ATOM | 996  | CZ  | ARG A 138 | 0.914  | 20.863 | 43.499 | 1.00 | 47.95 | C |
| ATOM | 997  | NH1 | ARG A 138 | 1.262  | 19.627 | 43.162 | 1.00 | 49.02 | N |
| ATOM | 998  | NH2 | ARG A 138 | 1.864  | 21.767 | 43.709 | 1.00 | 47.70 | N |
| ATOM | 999  | N   | GLY A 139 | -4.450 | 21.569 | 39.143 | 1.00 | 42.62 | N |
| ATOM | 1000 | CA  | GLY A 139 | -4.371 | 22.871 | 38.504 | 1.00 | 41.93 | C |
| ATOM | 1001 | C   | GLY A 139 | -3.389 | 23.820 | 39.174 | 1.00 | 41.28 | C |
| ATOM | 1002 | O   | GLY A 139 | -3.607 | 25.030 | 39.196 | 1.00 | 41.58 | O |
| ATOM | 1003 | N   | GLY A 140 | -2.291 | 23.292 | 39.703 | 1.00 | 40.31 | N |
| ATOM | 1004 | CA  | GLY A 140 | -1.329 | 24.119 | 40.410 | 1.00 | 39.43 | C |
| ATOM | 1005 | C   | GLY A 140 | -0.563 | 25.070 | 39.512 | 1.00 | 38.71 | C |
| ATOM | 1006 | O   | GLY A 140 | -0.495 | 24.871 | 38.294 | 1.00 | 38.40 | O |
| ATOM | 1007 | N   | GLU A 141 | 0.003  | 26.117 | 40.110 | 1.00 | 37.82 | N |
| ATOM | 1008 | CA  | GLU A 141 | 0.829  | 27.066 | 39.363 | 1.00 | 37.20 | C |
| ATOM | 1009 | C   | GLU A 141 | 2.320  | 26.726 | 39.491 | 1.00 | 35.94 | C |
| ATOM | 1010 | O   | GLU A 141 | 3.160  | 27.356 | 38.845 | 1.00 | 35.76 | O |
| ATOM | 1011 | CB  | GLU A 141 | 0.590  | 28.510 | 39.828 | 1.00 | 37.63 | C |
| ATOM | 1012 | CG  | GLU A 141 | -0.729 | 29.146 | 39.379 | 1.00 | 39.51 | C |
| ATOM | 1013 | CD  | GLU A 141 | -0.936 | 29.164 | 37.866 | 1.00 | 41.63 | C |
| ATOM | 1014 | OE1 | GLU A 141 | 0.056  | 29.147 | 37.102 | 1.00 | 42.42 | O |
| ATOM | 1015 | OE2 | GLU A 141 | -2.115 | 29.202 | 37.434 | 1.00 | 43.77 | O |
| ATOM | 1016 | N   | GLU A 142 | 2.652  | 25.742 | 40.326 | 1.00 | 34.29 | N |
| ATOM | 1017 | CA  | GLU A 142 | 4.045  | 25.351 | 40.510 | 1.00 | 33.08 | C |
| ATOM | 1018 | C   | GLU A 142 | 4.655  | 24.938 | 39.170 | 1.00 | 31.87 | C |
| ATOM | 1019 | O   | GLU A 142 | 3.958  | 24.443 | 38.296 | 1.00 | 31.87 | O |
| ATOM | 1020 | CB  | GLU A 142 | 4.170  | 24.201 | 41.519 | 1.00 | 32.96 | C |
| ATOM | 1021 | CG  | GLU A 142 | 5.610  | 23.914 | 41.942 | 1.00 | 32.71 | C |
| ATOM | 1022 | CD  | GLU A 142 | 5.761  | 22.730 | 42.896 | 1.00 | 33.55 | C |
| ATOM | 1023 | OE1 | GLU A 142 | 4.778  | 22.001 | 43.146 | 1.00 | 32.41 | O |
| ATOM | 1024 | OE2 | GLU A 142 | 6.888  | 22.520 | 43.398 | 1.00 | 34.13 | O |
| ATOM | 1025 | N   | ARG A 143 | 5.954  | 25.156 | 39.017 | 1.00 | 30.56 | N |
| ATOM | 1026 | CA  | ARG A 143 | 6.662  | 24.766 | 37.803 | 1.00 | 29.79 | C |
| ATOM | 1027 | C   | ARG A 143 | 7.878  | 23.939 | 38.142 | 1.00 | 28.70 | C |
| ATOM | 1028 | O   | ARG A 143 | 8.565  | 24.210 | 39.127 | 1.00 | 28.88 | O |
| ATOM | 1029 | CB  | ARG A 143 | 7.142  | 25.991 | 37.040 | 1.00 | 29.90 | C |
| ATOM | 1030 | CG  | ARG A 143 | 6.043  | 26.832 | 36.441 | 1.00 | 30.80 | C |
| ATOM | 1031 | CD  | ARG A 143 | 6.591  | 27.992 | 35.636 | 1.00 | 30.70 | C |
| ATOM | 1032 | NE  | ARG A 143 | 5.538  | 28.715 | 34.935 | 1.00 | 30.86 | N |
| ATOM | 1033 | CZ  | ARG A 143 | 5.168  | 28.487 | 33.682 | 1.00 | 29.53 | C |
| ATOM | 1034 | NH1 | ARG A 143 | 5.763  | 27.547 | 32.941 | 1.00 | 27.51 | N |
| ATOM | 1035 | NH2 | ARG A 143 | 4.196  | 29.216 | 33.168 | 1.00 | 30.04 | N |
| ATOM | 1036 | N   | LEU A 144 | 8.156  | 22.943 | 37.315 | 1.00 | 27.27 | N |
| ATOM | 1037 | CA  | LEU A 144 | 9.319  | 22.102 | 37.518 | 1.00 | 26.47 | C |
| ATOM | 1038 | C   | LEU A 144 | 10.220 | 22.148 | 36.297 | 1.00 | 25.40 | C |
| ATOM | 1039 | O   | LEU A 144 | 9.755  | 22.330 | 35.172 | 1.00 | 25.39 | O |
| ATOM | 1040 | CB  | LEU A 144 | 8.893  | 20.652 | 37.753 | 1.00 | 26.70 | C |
| ATOM | 1041 | CG  | LEU A 144 | 7.922  | 20.416 | 38.915 | 1.00 | 27.15 | C |
| ATOM | 1042 | CD1 | LEU A 144 | 7.575  | 18.921 | 39.059 | 1.00 | 27.40 | C |
| ATOM | 1043 | CD2 | LEU A 144 | 8.488  | 20.956 | 40.221 | 1.00 | 27.42 | C |
| ATOM | 1044 | N   | TYR A 145 | 11.511 | 21.974 | 36.527 | 1.00 | 23.90 | N |
| ATOM | 1045 | CA  | TYR A 145 | 12.458 | 21.871 | 35.441 | 1.00 | 23.15 | C |
| ATOM | 1046 | C   | TYR A 145 | 13.516 | 20.857 | 35.868 | 1.00 | 23.04 | C |
| ATOM | 1047 | O   | TYR A 145 | 14.328 | 21.130 | 36.740 | 1.00 | 22.58 | O |
| ATOM | 1048 | CB  | TYR A 145 | 13.080 | 23.235 | 35.107 | 1.00 | 23.01 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1049 | CG  | TYR | A | 145 | 13.522 | 23.419 | 33.666 | 1.00 | 21.34 | C |
| ATOM | 1050 | CD1 | TYR | A | 145 | 13.824 | 22.333 | 32.863 | 1.00 | 20.11 | C |
| ATOM | 1051 | CD2 | TYR | A | 145 | 13.662 | 24.691 | 33.119 | 1.00 | 21.14 | C |
| ATOM | 1052 | CE1 | TYR | A | 145 | 14.219 | 22.494 | 31.563 | 1.00 | 20.22 | C |
| ATOM | 1053 | CE2 | TYR | A | 145 | 14.075 | 24.866 | 31.807 | 1.00 | 19.81 | C |
| ATOM | 1054 | CZ  | TYR | A | 145 | 14.349 | 23.764 | 31.027 | 1.00 | 19.19 | C |
| ATOM | 1055 | OH  | TYR | A | 145 | 14.736 | 23.903 | 29.699 | 1.00 | 18.36 | O |
| ATOM | 1056 | N   | LEU | A | 146 | 13.461 | 19.666 | 35.287 | 1.00 | 22.75 | N |
| ATOM | 1057 | CA  | LEU | A | 146 | 14.490 | 18.661 | 35.516 | 1.00 | 23.17 | C |
| ATOM | 1058 | C   | LEU | A | 146 | 15.720 | 19.005 | 34.679 | 1.00 | 22.99 | C |
| ATOM | 1059 | O   | LEU | A | 146 | 15.604 | 19.264 | 33.490 | 1.00 | 22.81 | O |
| ATOM | 1060 | CB  | LEU | A | 146 | 13.980 | 17.282 | 35.115 | 1.00 | 23.33 | C |
| ATOM | 1061 | CG  | LEU | A | 146 | 14.992 | 16.141 | 35.274 | 1.00 | 24.98 | C |
| ATOM | 1062 | CD1 | LEU | A | 146 | 14.276 | 14.846 | 35.622 | 1.00 | 24.56 | C |
| ATOM | 1063 | CD2 | LEU | A | 146 | 15.849 | 15.946 | 34.016 | 1.00 | 26.13 | C |
| ATOM | 1064 | N   | GLN | A | 147 | 16.891 | 18.983 | 35.299 | 1.00 | 23.05 | N |
| ATOM | 1065 | CA  | GLN | A | 147 | 18.135 | 19.314 | 34.619 | 1.00 | 23.65 | C |
| ATOM | 1066 | C   | GLN | A | 147 | 19.158 | 18.394 | 35.231 | 1.00 | 23.86 | C |
| ATOM | 1067 | O   | GLN | A | 147 | 19.573 | 18.597 | 36.364 | 1.00 | 24.61 | O |
| ATOM | 1068 | CB  | GLN | A | 147 | 18.516 | 20.793 | 34.821 | 1.00 | 23.53 | C |
| ATOM | 1069 | CG  | GLN | A | 147 | 17.386 | 21.770 | 34.461 | 1.00 | 24.34 | C |
| ATOM | 1070 | CD  | GLN | A | 147 | 17.800 | 23.238 | 34.482 | 1.00 | 26.20 | C |
| ATOM | 1071 | OE1 | GLN | A | 147 | 17.034 | 24.114 | 34.035 | 1.00 | 29.67 | O |
| ATOM | 1072 | NE2 | GLN | A | 147 | 18.979 | 23.514 | 34.988 | 1.00 | 21.33 | N |
| ATOM | 1073 | N   | GLN | A | 148 | 19.542 | 17.369 | 34.485 | 1.00 | 24.35 | N |
| ATOM | 1074 | CA  | GLN | A | 148 | 20.393 | 16.314 | 35.006 | 1.00 | 24.70 | C |
| ATOM | 1075 | C   | GLN | A | 148 | 21.319 | 15.753 | 33.964 | 1.00 | 25.16 | C |
| ATOM | 1076 | O   | GLN | A | 148 | 20.898 | 15.378 | 32.866 | 1.00 | 24.21 | O |
| ATOM | 1077 | CB  | GLN | A | 148 | 19.525 | 15.172 | 35.526 | 1.00 | 24.97 | C |
| ATOM | 1078 | CG  | GLN | A | 148 | 20.317 | 13.940 | 35.953 | 1.00 | 25.54 | C |
| ATOM | 1079 | CD  | GLN | A | 148 | 21.275 | 14.256 | 37.085 | 1.00 | 26.98 | C |
| ATOM | 1080 | OE1 | GLN | A | 148 | 20.892 | 14.941 | 38.042 | 1.00 | 26.73 | O |
| ATOM | 1081 | NE2 | GLN | A | 148 | 22.522 | 13.786 | 36.976 | 1.00 | 26.37 | N |
| ATOM | 1082 | N   | THR | A | 149 | 22.592 | 15.704 | 34.321 | 1.00 | 25.94 | N |
| ATOM | 1083 | CA  | THR | A | 149 | 23.603 | 15.134 | 33.466 | 1.00 | 27.43 | C |
| ATOM | 1084 | C   | THR | A | 149 | 23.369 | 13.632 | 33.324 | 1.00 | 27.29 | C |
| ATOM | 1085 | O   | THR | A | 149 | 23.081 | 12.965 | 34.303 | 1.00 | 27.40 | O |
| ATOM | 1086 | CB  | THR | A | 149 | 24.990 | 15.430 | 34.075 | 1.00 | 27.91 | C |
| ATOM | 1087 | OG1 | THR | A | 149 | 25.282 | 16.829 | 33.901 | 1.00 | 30.41 | O |
| ATOM | 1088 | CG2 | THR | A | 149 | 26.078 | 14.776 | 33.276 | 1.00 | 30.12 | C |
| ATOM | 1089 | N   | LEU | A | 150 | 23.461 | 13.117 | 32.100 | 1.00 | 27.79 | N |
| ATOM | 1090 | CA  | LEU | A | 150 | 23.321 | 11.690 | 31.832 | 1.00 | 28.02 | C |
| ATOM | 1091 | C   | LEU | A | 150 | 24.549 | 10.935 | 32.364 | 1.00 | 28.42 | C |
| ATOM | 1092 | O   | LEU | A | 150 | 25.682 | 11.261 | 32.002 | 1.00 | 28.86 | O |
| ATOM | 1093 | CB  | LEU | A | 150 | 23.194 | 11.435 | 30.326 | 1.00 | 28.08 | C |
| ATOM | 1094 | CG  | LEU | A | 150 | 21.929 | 11.937 | 29.622 | 1.00 | 28.70 | C |
| ATOM | 1095 | CD1 | LEU | A | 150 | 22.016 | 11.725 | 28.117 | 1.00 | 28.62 | C |
| ATOM | 1096 | CD2 | LEU | A | 150 | 20.697 | 11.260 | 30.175 | 1.00 | 29.47 | C |
| ATOM | 1097 | N   | ASN | A | 151 | 24.332 | 9.928  | 33.203 | 1.00 | 28.58 | N |
| ATOM | 1098 | CA  | ASN | A | 151 | 25.434 | 9.156  | 33.781 | 1.00 | 28.79 | C |
| ATOM | 1099 | C   | ASN | A | 151 | 25.194 | 7.636  | 33.782 | 1.00 | 29.24 | C |
| ATOM | 1100 | O   | ASN | A | 151 | 24.197 | 7.163  | 33.238 | 1.00 | 29.60 | O |
| ATOM | 1101 | CB  | ASN | A | 151 | 25.657 | 9.631  | 35.208 | 1.00 | 28.77 | C |
| ATOM | 1102 | CG  | ASN | A | 151 | 24.459 | 9.367  | 36.084 | 1.00 | 28.05 | C |
| ATOM | 1103 | OD1 | ASN | A | 151 | 23.936 | 8.246  | 36.126 | 1.00 | 29.02 | O |
| ATOM | 1104 | ND2 | ASN | A | 151 | 24.000 | 10.396 | 36.772 | 1.00 | 26.99 | N |
| ATOM | 1105 | N   | ASP | A | 152 | 26.083 | 6.885  | 34.437 | 1.00 | 29.71 | N |
| ATOM | 1106 | CA  | ASP | A | 152 | 26.039 | 5.410  | 34.448 | 1.00 | 30.06 | C |
| ATOM | 1107 | C   | ASP | A | 152 | 24.850 | 4.733  | 35.075 | 1.00 | 29.51 | C |
| ATOM | 1108 | O   | ASP | A | 152 | 24.771 | 3.503  | 35.026 | 1.00 | 28.98 | O |
| ATOM | 1109 | CB  | ASP | A | 152 | 27.199 | 4.829  | 35.250 | 1.00 | 30.99 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1110 | CG  | ASP | A | 152 | 28.447 | 5.561  | 35.048 | 1.00 | 33.80 | C |
| ATOM | 1111 | OD1 | ASP | A | 152 | 28.636 | 6.071  | 33.918 | 1.00 | 40.13 | O |
| ATOM | 1112 | OD2 | ASP | A | 152 | 29.274 | 5.719  | 35.960 | 1.00 | 35.65 | O |
| ATOM | 1113 | N   | THR | A | 153 | 23.959 | 5.468  | 35.722 | 1.00 | 28.96 | N |
| ATOM | 1114 | CA  | THR | A | 153 | 22.831 | 4.792  | 36.359 | 1.00 | 28.42 | C |
| ATOM | 1115 | C   | THR | A | 153 | 21.685 | 4.594  | 35.387 | 1.00 | 27.75 | C |
| ATOM | 1116 | O   | THR | A | 153 | 20.730 | 3.909  | 35.712 | 1.00 | 27.68 | O |
| ATOM | 1117 | CB  | THR | A | 153 | 22.330 | 5.552  | 37.584 | 1.00 | 28.53 | C |
| ATOM | 1118 | OG1 | THR | A | 153 | 21.833 | 6.836  | 37.193 | 1.00 | 28.91 | O |
| ATOM | 1119 | CG2 | THR | A | 153 | 23.473 | 5.855  | 38.540 | 1.00 | 29.18 | C |
| ATOM | 1120 | N   | VAL | A | 154 | 21.766 | 5.171  | 34.194 | 1.00 | 26.76 | N |
| ATOM | 1121 | CA  | VAL | A | 154 | 20.671 | 4.996  | 33.246 | 1.00 | 26.61 | C |
| ATOM | 1122 | C   | VAL | A | 154 | 20.583 | 3.531  | 32.895 | 1.00 | 26.77 | C |
| ATOM | 1123 | O   | VAL | A | 154 | 21.592 | 2.832  | 32.923 | 1.00 | 27.36 | O |
| ATOM | 1124 | CB  | VAL | A | 154 | 20.838 | 5.826  | 31.964 | 1.00 | 26.05 | C |
| ATOM | 1125 | CG1 | VAL | A | 154 | 20.914 | 7.279  | 32.312 | 1.00 | 26.14 | C |
| ATOM | 1126 | CG2 | VAL | A | 154 | 22.071 | 5.383  | 31.182 | 1.00 | 25.62 | C |
| ATOM | 1127 | N   | GLY | A | 155 | 19.379 | 3.072  | 32.568 | 1.00 | 26.71 | N |
| ATOM | 1128 | CA  | GLY | A | 155 | 19.147 | 1.674  | 32.252 | 1.00 | 26.42 | C |
| ATOM | 1129 | C   | GLY | A | 155 | 19.531 | 1.266  | 30.840 | 1.00 | 26.67 | C |
| ATOM | 1130 | O   | GLY | A | 155 | 19.894 | 2.093  | 29.983 | 1.00 | 26.52 | O |
| ATOM | 1131 | N   | ARG | A | 156 | 19.390 | -0.028 | 30.599 | 1.00 | 26.49 | N |
| ATOM | 1132 | CA  | ARG | A | 156 | 19.811 | -0.684 | 29.364 | 1.00 | 26.54 | C |
| ATOM | 1133 | C   | ARG | A | 156 | 19.305 | -0.053 | 28.068 | 1.00 | 25.95 | C |
| ATOM | 1134 | O   | ARG | A | 156 | 20.089 | 0.194  | 27.160 | 1.00 | 26.26 | O |
| ATOM | 1135 | CB  | ARG | A | 156 | 19.429 | -2.165 | 29.418 | 1.00 | 26.28 | C |
| ATOM | 1136 | N   | LYS | A | 157 | 18.004 | 0.175  | 27.964 | 1.00 | 25.43 | N |
| ATOM | 1137 | CA  | LYS | A | 157 | 17.460 | 0.777  | 26.756 | 1.00 | 25.11 | C |
| ATOM | 1138 | C   | LYS | A | 157 | 18.026 | 2.198  | 26.517 | 1.00 | 25.50 | C |
| ATOM | 1139 | O   | LYS | A | 157 | 18.249 | 2.595  | 25.372 | 1.00 | 25.14 | O |
| ATOM | 1140 | CB  | LYS | A | 157 | 15.927 | 0.796  | 26.809 | 1.00 | 24.88 | C |
| ATOM | 1141 | CG  | LYS | A | 157 | 15.255 | -0.572 | 26.516 | 1.00 | 24.25 | C |
| ATOM | 1142 | N   | ILE | A | 158 | 18.257 | 2.956  | 27.585 | 1.00 | 25.35 | N |
| ATOM | 1143 | CA  | ILE | A | 158 | 18.766 | 4.326  | 27.432 | 1.00 | 25.61 | C |
| ATOM | 1144 | C   | ILE | A | 158 | 20.205 | 4.250  | 26.971 | 1.00 | 25.76 | C |
| ATOM | 1145 | O   | ILE | A | 158 | 20.661 | 5.058  | 26.166 | 1.00 | 25.39 | O |
| ATOM | 1146 | CB  | ILE | A | 158 | 18.662 | 5.107  | 28.740 | 1.00 | 25.41 | C |
| ATOM | 1147 | CG1 | ILE | A | 158 | 17.202 | 5.245  | 29.162 | 1.00 | 25.92 | C |
| ATOM | 1148 | CG2 | ILE | A | 158 | 19.297 | 6.475  | 28.601 | 1.00 | 25.61 | C |
| ATOM | 1149 | CD1 | ILE | A | 158 | 16.331 | 5.924  | 28.174 | 1.00 | 27.88 | C |
| ATOM | 1150 | N   | VAL | A | 159 | 20.909 | 3.251  | 27.481 | 1.00 | 26.10 | N |
| ATOM | 1151 | CA  | VAL | A | 159 | 22.276 | 3.010  | 27.079 | 1.00 | 26.57 | C |
| ATOM | 1152 | C   | VAL | A | 159 | 22.279 | 2.703  | 25.585 | 1.00 | 26.40 | C |
| ATOM | 1153 | O   | VAL | A | 159 | 23.074 | 3.248  | 24.840 | 1.00 | 26.32 | O |
| ATOM | 1154 | CB  | VAL | A | 159 | 22.895 | 1.850  | 27.883 | 1.00 | 26.94 | C |
| ATOM | 1155 | CG1 | VAL | A | 159 | 24.136 | 1.310  | 27.193 | 1.00 | 27.73 | C |
| ATOM | 1156 | CG2 | VAL | A | 159 | 23.223 | 2.308  | 29.298 | 1.00 | 26.73 | C |
| ATOM | 1157 | N   | MET | A | 160 | 21.363 | 1.852  | 25.145 | 1.00 | 26.48 | N |
| ATOM | 1158 | CA  | MET | A | 160 | 21.270 | 1.518  | 23.721 | 1.00 | 26.52 | C |
| ATOM | 1159 | C   | MET | A | 160 | 20.985 | 2.771  | 22.880 | 1.00 | 25.02 | C |
| ATOM | 1160 | O   | MET | A | 160 | 21.600 | 2.986  | 21.845 | 1.00 | 24.31 | O |
| ATOM | 1161 | CB  | MET | A | 160 | 20.183 | 0.476  | 23.485 | 1.00 | 27.05 | C |
| ATOM | 1162 | CG  | MET | A | 160 | 20.540 | -0.900 | 24.001 | 1.00 | 30.45 | C |
| ATOM | 1163 | SD  | MET | A | 160 | 21.843 | -1.730 | 23.058 | 1.00 | 34.87 | S |
| ATOM | 1164 | CE  | MET | A | 160 | 20.957 | -2.028 | 21.496 | 1.00 | 36.94 | C |
| ATOM | 1165 | N   | ASP | A | 161 | 20.047 | 3.589  | 23.342 | 1.00 | 23.96 | N |
| ATOM | 1166 | CA  | ASP | A | 161 | 19.699 | 4.831  | 22.665 | 1.00 | 23.14 | C |
| ATOM | 1167 | C   | ASP | A | 161 | 20.890 | 5.781  | 22.550 | 1.00 | 21.93 | C |
| ATOM | 1168 | O   | ASP | A | 161 | 21.167 | 6.323  | 21.480 | 1.00 | 21.41 | O |
| ATOM | 1169 | CB  | ASP | A | 161 | 18.549 | 5.528  | 23.402 | 1.00 | 23.13 | C |
| ATOM | 1170 | CG  | ASP | A | 161 | 17.250 | 4.762  | 23.293 | 1.00 | 24.08 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1171 | OD1 | ASP | A | 161 | 17.182 | 3.812  | 22.478 | 1.00 | 21.27 | O |
| ATOM | 1172 | OD2 | ASP | A | 161 | 16.248 | 5.035  | 23.980 | 1.00 | 25.87 | O |
| ATOM | 1173 | N   | PHE | A | 162 | 21.575 | 5.973  | 23.671 | 1.00 | 20.59 | N |
| ATOM | 1174 | CA  | PHE | A | 162 | 22.712 | 6.859  | 23.765 | 1.00 | 19.97 | C |
| ATOM | 1175 | C   | PHE | A | 162 | 23.802 | 6.409  | 22.809 | 1.00 | 19.19 | C |
| ATOM | 1176 | O   | PHE | A | 162 | 24.410 | 7.213  | 22.160 | 1.00 | 18.98 | O |
| ATOM | 1177 | CB  | PHE | A | 162 | 23.223 | 6.859  | 25.220 | 1.00 | 20.44 | C |
| ATOM | 1178 | CG  | PHE | A | 162 | 24.386 | 7.755  | 25.470 | 1.00 | 20.78 | C |
| ATOM | 1179 | CD1 | PHE | A | 162 | 24.206 | 9.107  | 25.673 | 1.00 | 25.50 | C |
| ATOM | 1180 | CD2 | PHE | A | 162 | 25.662 | 7.245  | 25.542 | 1.00 | 23.71 | C |
| ATOM | 1181 | CE1 | PHE | A | 162 | 25.290 | 9.930  | 25.935 | 1.00 | 25.85 | C |
| ATOM | 1182 | CE2 | PHE | A | 162 | 26.755 | 8.072  | 25.795 | 1.00 | 24.89 | C |
| ATOM | 1183 | CZ  | PHE | A | 162 | 26.572 | 9.394  | 26.001 | 1.00 | 23.50 | C |
| ATOM | 1184 | N   | LEU | A | 163 | 24.062 | 5.115  | 22.744 | 1.00 | 19.25 | N |
| ATOM | 1185 | CA  | LEU | A | 163 | 25.084 | 4.597  | 21.838 | 1.00 | 19.42 | C |
| ATOM | 1186 | C   | LEU | A | 163 | 24.715 | 4.804  | 20.361 | 1.00 | 18.63 | C |
| ATOM | 1187 | O   | LEU | A | 163 | 25.585 | 4.831  | 19.493 | 1.00 | 18.21 | O |
| ATOM | 1188 | CB  | LEU | A | 163 | 25.297 | 3.115  | 22.104 | 1.00 | 19.49 | C |
| ATOM | 1189 | CG  | LEU | A | 163 | 25.988 | 2.812  | 23.422 | 1.00 | 20.88 | C |
| ATOM | 1190 | CD1 | LEU | A | 163 | 25.980 | 1.319  | 23.651 | 1.00 | 22.44 | C |
| ATOM | 1191 | CD2 | LEU | A | 163 | 27.407 | 3.368  | 23.396 | 1.00 | 21.73 | C |
| ATOM | 1192 | N   | GLY | A | 164 | 23.419 | 4.917  | 20.104 | 1.00 | 18.01 | N |
| ATOM | 1193 | CA  | GLY | A | 164 | 22.889 | 5.158  | 18.779 | 1.00 | 18.55 | C |
| ATOM | 1194 | C   | GLY | A | 164 | 22.873 | 6.622  | 18.355 | 1.00 | 18.40 | C |
| ATOM | 1195 | O   | GLY | A | 164 | 22.406 | 6.921  | 17.256 | 1.00 | 19.24 | O |
| ATOM | 1196 | N   | PHE | A | 165 | 23.365 | 7.521  | 19.209 | 1.00 | 17.50 | N |
| ATOM | 1197 | CA  | PHE | A | 165 | 23.493 | 8.913  | 18.831 | 1.00 | 17.67 | C |
| ATOM | 1198 | C   | PHE | A | 165 | 24.497 | 8.955  | 17.663 | 1.00 | 17.49 | C |
| ATOM | 1199 | O   | PHE | A | 165 | 25.293 | 8.028  | 17.497 | 1.00 | 16.10 | O |
| ATOM | 1200 | CB  | PHE | A | 165 | 23.984 | 9.753  | 20.018 | 1.00 | 17.47 | C |
| ATOM | 1201 | CG  | PHE | A | 165 | 22.932 | 10.004 | 21.098 | 1.00 | 18.51 | C |
| ATOM | 1202 | CD1 | PHE | A | 165 | 21.645 | 9.479  | 21.009 | 1.00 | 19.26 | C |
| ATOM | 1203 | CD2 | PHE | A | 165 | 23.242 | 10.784 | 22.203 | 1.00 | 18.52 | C |
| ATOM | 1204 | CE1 | PHE | A | 165 | 20.697 | 9.730  | 21.996 | 1.00 | 18.44 | C |
| ATOM | 1205 | CE2 | PHE | A | 165 | 22.303 | 11.030 | 23.199 | 1.00 | 18.52 | C |
| ATOM | 1206 | CZ  | PHE | A | 165 | 21.032 | 10.500 | 23.100 | 1.00 | 18.90 | C |
| ATOM | 1207 | N   | ASN | A | 166 | 24.466 | 10.009 | 16.854 | 1.00 | 17.77 | N |
| ATOM | 1208 | CA  | ASN | A | 166 | 25.393 | 10.110 | 15.712 | 1.00 | 18.29 | C |
| ATOM | 1209 | C   | ASN | A | 166 | 26.787 | 10.622 | 16.129 | 1.00 | 18.73 | C |
| ATOM | 1210 | O   | ASN | A | 166 | 27.156 | 11.795 | 15.897 | 1.00 | 19.54 | O |
| ATOM | 1211 | CB  | ASN | A | 166 | 24.793 | 10.972 | 14.598 | 1.00 | 17.92 | C |
| ATOM | 1212 | CG  | ASN | A | 166 | 25.571 | 10.861 | 13.293 | 1.00 | 17.28 | C |
| ATOM | 1213 | OD1 | ASN | A | 166 | 26.679 | 10.289 | 13.262 | 1.00 | 16.53 | O |
| ATOM | 1214 | ND2 | ASN | A | 166 | 24.994 | 11.395 | 12.204 | 1.00 | 12.92 | N |
| ATOM | 1215 | N   | TRP | A | 167 | 27.527 | 9.739  | 16.789 | 1.00 | 19.26 | N |
| ATOM | 1216 | CA  | TRP | A | 167 | 28.867 | 10.035 | 17.264 | 1.00 | 19.76 | C |
| ATOM | 1217 | C   | TRP | A | 167 | 29.785 | 10.266 | 16.084 | 1.00 | 19.88 | C |
| ATOM | 1218 | O   | TRP | A | 167 | 30.731 | 11.031 | 16.169 | 1.00 | 19.35 | O |
| ATOM | 1219 | CB  | TRP | A | 167 | 29.384 | 8.864  | 18.130 | 1.00 | 19.92 | C |
| ATOM | 1220 | CG  | TRP | A | 167 | 28.556 | 8.728  | 19.351 | 1.00 | 20.39 | C |
| ATOM | 1221 | CD1 | TRP | A | 167 | 27.686 | 7.727  | 19.656 | 1.00 | 20.85 | C |
| ATOM | 1222 | CD2 | TRP | A | 167 | 28.445 | 9.686  | 20.400 | 1.00 | 20.99 | C |
| ATOM | 1223 | NE1 | TRP | A | 167 | 27.059 | 7.995  | 20.851 | 1.00 | 21.18 | N |
| ATOM | 1224 | CE2 | TRP | A | 167 | 27.509 | 9.194  | 21.325 | 1.00 | 20.70 | C |
| ATOM | 1225 | CE3 | TRP | A | 167 | 29.065 | 10.916 | 20.664 | 1.00 | 21.55 | C |
| ATOM | 1226 | CZ2 | TRP | A | 167 | 27.183 | 9.871  | 22.488 | 1.00 | 22.63 | C |
| ATOM | 1227 | CZ3 | TRP | A | 167 | 28.731 | 11.589 | 21.804 | 1.00 | 21.78 | C |
| ATOM | 1228 | CH2 | TRP | A | 167 | 27.789 | 11.071 | 22.706 | 1.00 | 22.79 | C |
| ATOM | 1229 | N   | ASN | A | 168 | 29.529 | 9.577  | 14.979 | 1.00 | 20.07 | N |
| ATOM | 1230 | CA  | ASN | A | 168 | 30.374 | 9.759  | 13.818 | 1.00 | 20.50 | C |
| ATOM | 1231 | C   | ASN | A | 168 | 30.396 | 11.237 | 13.421 | 1.00 | 20.67 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1232 | O   | ASN | A | 168 | 31.465 | 11.806 | 13.207 | 1.00 | 19.54 | O |
| ATOM | 1233 | CB  | ASN | A | 168 | 29.917 | 8.930  | 12.628 | 1.00 | 20.87 | C |
| ATOM | 1234 | CG  | ASN | A | 168 | 30.818 | 9.129  | 11.423 | 1.00 | 22.96 | C |
| ATOM | 1235 | OD1 | ASN | A | 168 | 32.027 | 8.923  | 11.522 | 1.00 | 25.54 | O |
| ATOM | 1236 | ND2 | ASN | A | 168 | 30.247 | 9.578  | 10.295 | 1.00 | 23.09 | N |
| ATOM | 1237 | N   | TRP | A | 169 | 29.211 | 11.844 | 13.338 | 1.00 | 20.57 | N |
| ATOM | 1238 | CA  | TRP | A | 169 | 29.106 | 13.226 | 12.917 | 1.00 | 20.23 | C |
| ATOM | 1239 | C   | TRP | A | 169 | 29.653 | 14.188 | 13.972 | 1.00 | 20.59 | C |
| ATOM | 1240 | O   | TRP | A | 169 | 30.367 | 15.118 | 13.634 | 1.00 | 20.09 | O |
| ATOM | 1241 | CB  | TRP | A | 169 | 27.662 | 13.618 | 12.570 | 1.00 | 20.35 | C |
| ATOM | 1242 | CG  | TRP | A | 169 | 27.542 | 15.101 | 12.238 | 1.00 | 19.49 | C |
| ATOM | 1243 | CD1 | TRP | A | 169 | 27.769 | 15.693 | 11.026 | 1.00 | 19.03 | C |
| ATOM | 1244 | CD2 | TRP | A | 169 | 27.203 | 16.157 | 13.137 | 1.00 | 20.25 | C |
| ATOM | 1245 | NE1 | TRP | A | 169 | 27.578 | 17.052 | 11.117 | 1.00 | 20.36 | N |
| ATOM | 1246 | CE2 | TRP | A | 169 | 27.244 | 17.366 | 12.406 | 1.00 | 19.45 | C |
| ATOM | 1247 | CE3 | TRP | A | 169 | 26.874 | 16.207 | 14.492 | 1.00 | 20.60 | C |
| ATOM | 1248 | CZ2 | TRP | A | 169 | 26.964 | 18.600 | 12.975 | 1.00 | 21.03 | C |
| ATOM | 1249 | CZ3 | TRP | A | 169 | 26.614 | 17.433 | 15.064 | 1.00 | 23.09 | C |
| ATOM | 1250 | CH2 | TRP | A | 169 | 26.649 | 18.621 | 14.297 | 1.00 | 23.61 | C |
| ATOM | 1251 | N   | ILE | A | 170 | 29.326 | 13.979 | 15.239 | 1.00 | 20.47 | N |
| ATOM | 1252 | CA  | ILE | A | 170 | 29.759 | 14.926 | 16.241 | 1.00 | 20.67 | C |
| ATOM | 1253 | C   | ILE | A | 170 | 31.262 | 14.772 | 16.567 | 1.00 | 21.18 | C |
| ATOM | 1254 | O   | ILE | A | 170 | 31.943 | 15.758 | 16.836 | 1.00 | 21.20 | O |
| ATOM | 1255 | CB  | ILE | A | 170 | 28.842 | 14.892 | 17.483 | 1.00 | 20.61 | C |
| ATOM | 1256 | CG1 | ILE | A | 170 | 28.900 | 16.231 | 18.221 | 1.00 | 20.05 | C |
| ATOM | 1257 | CG2 | ILE | A | 170 | 29.191 | 13.755 | 18.402 | 1.00 | 19.89 | C |
| ATOM | 1258 | CD1 | ILE | A | 170 | 27.865 | 16.353 | 19.329 | 1.00 | 21.00 | C |
| ATOM | 1259 | N   | ASN | A | 171 | 31.780 | 13.556 | 16.527 | 1.00 | 20.74 | N |
| ATOM | 1260 | CA  | ASN | A | 171 | 33.214 | 13.355 | 16.715 | 1.00 | 21.80 | C |
| ATOM | 1261 | C   | ASN | A | 171 | 34.024 | 14.093 | 15.634 | 1.00 | 22.34 | C |
| ATOM | 1262 | O   | ASN | A | 171 | 35.093 | 14.652 | 15.916 | 1.00 | 21.98 | O |
| ATOM | 1263 | CB  | ASN | A | 171 | 33.581 | 11.857 | 16.718 | 1.00 | 21.55 | C |
| ATOM | 1264 | CG  | ASN | A | 171 | 33.111 | 11.124 | 17.981 | 1.00 | 21.20 | C |
| ATOM | 1265 | OD1 | ASN | A | 171 | 32.637 | 11.724 | 18.963 | 1.00 | 21.35 | O |
| ATOM | 1266 | ND2 | ASN | A | 171 | 33.263 | 9.830  | 17.962 | 1.00 | 19.36 | N |
| ATOM | 1267 | N   | LYS | A | 172 | 33.529 | 14.097 | 14.400 | 1.00 | 22.97 | N |
| ATOM | 1268 | CA  | LYS | A | 172 | 34.218 | 14.847 | 13.353 | 1.00 | 24.09 | C |
| ATOM | 1269 | C   | LYS | A | 172 | 34.167 | 16.342 | 13.656 | 1.00 | 23.61 | C |
| ATOM | 1270 | O   | LYS | A | 172 | 35.166 | 17.041 | 13.511 | 1.00 | 23.54 | O |
| ATOM | 1271 | CB  | LYS | A | 172 | 33.669 | 14.529 | 11.961 | 1.00 | 24.58 | C |
| ATOM | 1272 | CG  | LYS | A | 172 | 34.087 | 13.163 | 11.491 | 1.00 | 27.56 | C |
| ATOM | 1273 | CD  | LYS | A | 172 | 33.653 | 12.852 | 10.034 | 1.00 | 31.03 | C |
| ATOM | 1274 | CE  | LYS | A | 172 | 34.323 | 11.576 | 9.565  | 1.00 | 33.01 | C |
| ATOM | 1275 | NZ  | LYS | A | 172 | 34.357 | 11.406 | 8.070  | 1.00 | 36.89 | N |
| ATOM | 1276 | N   | GLN | A | 173 | 33.019 | 16.834 | 14.109 | 1.00 | 23.74 | N |
| ATOM | 1277 | CA  | GLN | A | 173 | 32.914 | 18.245 | 14.482 | 1.00 | 23.87 | C |
| ATOM | 1278 | C   | GLN | A | 173 | 33.960 | 18.578 | 15.547 | 1.00 | 23.86 | C |
| ATOM | 1279 | O   | GLN | A | 173 | 34.739 | 19.500 | 15.374 | 1.00 | 24.25 | O |
| ATOM | 1280 | CB  | GLN | A | 173 | 31.517 | 18.590 | 14.993 | 1.00 | 23.63 | C |
| ATOM | 1281 | CG  | GLN | A | 173 | 30.451 | 18.619 | 13.916 | 1.00 | 24.53 | C |
| ATOM | 1282 | CD  | GLN | A | 173 | 30.753 | 19.634 | 12.851 | 1.00 | 25.08 | C |
| ATOM | 1283 | OE1 | GLN | A | 173 | 31.194 | 20.740 | 13.157 | 1.00 | 26.69 | O |
| ATOM | 1284 | NE2 | GLN | A | 173 | 30.512 | 19.273 | 11.601 | 1.00 | 23.36 | N |
| ATOM | 1285 | N   | GLN | A | 174 | 33.963 | 17.822 | 16.635 | 1.00 | 23.63 | N |
| ATOM | 1286 | CA  | GLN | A | 174 | 34.925 | 17.995 | 17.717 | 1.00 | 23.91 | C |
| ATOM | 1287 | C   | GLN | A | 174 | 36.365 | 18.053 | 17.161 | 1.00 | 24.01 | C |
| ATOM | 1288 | O   | GLN | A | 174 | 37.133 | 18.962 | 17.480 | 1.00 | 23.39 | O |
| ATOM | 1289 | CB  | GLN | A | 174 | 34.783 | 16.840 | 18.717 | 1.00 | 23.67 | C |
| ATOM | 1290 | CG  | GLN | A | 174 | 35.688 | 16.913 | 19.934 | 1.00 | 24.07 | C |
| ATOM | 1291 | CD  | GLN | A | 174 | 35.595 | 15.668 | 20.799 | 1.00 | 25.12 | C |
| ATOM | 1292 | OE1 | GLN | A | 174 | 35.229 | 14.602 | 20.312 | 1.00 | 25.70 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1293 | NE2 | GLN | A | 174 | 35.901 | 15.803 | 22.084 | 1.00 | 23.63 | N |
| ATOM | 1294 | N   | GLY | A | 175 | 36.706 | 17.080 | 16.334 | 1.00 | 23.75 | N |
| ATOM | 1295 | CA  | GLY | A | 175 | 38.005 | 17.028 | 15.696 | 1.00 | 24.73 | C |
| ATOM | 1296 | C   | GLY | A | 175 | 38.268 | 18.209 | 14.768 | 1.00 | 25.21 | C |
| ATOM | 1297 | O   | GLY | A | 175 | 39.310 | 18.842 | 14.854 | 1.00 | 25.60 | O |
| ATOM | 1298 | N   | LYS | A | 176 | 37.327 | 18.518 | 13.888 | 1.00 | 25.81 | N |
| ATOM | 1299 | CA  | LYS | A | 176 | 37.491 | 19.634 | 12.961 | 1.00 | 26.88 | C |
| ATOM | 1300 | C   | LYS | A | 176 | 37.719 | 20.997 | 13.638 | 1.00 | 26.95 | C |
| ATOM | 1301 | O   | LYS | A | 176 | 38.490 | 21.803 | 13.136 | 1.00 | 26.74 | O |
| ATOM | 1302 | CB  | LYS | A | 176 | 36.256 | 19.778 | 12.077 | 1.00 | 27.35 | C |
| ATOM | 1303 | CG  | LYS | A | 176 | 36.093 | 18.716 | 11.009 | 1.00 | 29.87 | C |
| ATOM | 1304 | CD  | LYS | A | 176 | 34.894 | 19.085 | 10.137 | 1.00 | 33.21 | C |
| ATOM | 1305 | CE  | LYS | A | 176 | 33.948 | 17.932 | 9.961  | 1.00 | 35.30 | C |
| ATOM | 1306 | NZ  | LYS | A | 176 | 32.558 | 18.388 | 9.643  | 1.00 | 37.22 | N |
| ATOM | 1307 | N   | ARG | A | 177 | 37.031 | 21.257 | 14.749 | 1.00 | 26.93 | N |
| ATOM | 1308 | CA  | ARG | A | 177 | 37.153 | 22.539 | 15.435 | 1.00 | 27.36 | C |
| ATOM | 1309 | C   | ARG | A | 177 | 38.241 | 22.611 | 16.509 | 1.00 | 26.63 | C |
| ATOM | 1310 | O   | ARG | A | 177 | 38.402 | 23.650 | 17.135 | 1.00 | 25.85 | O |
| ATOM | 1311 | CB  | ARG | A | 177 | 35.832 | 22.902 | 16.114 | 1.00 | 27.86 | C |
| ATOM | 1312 | CG  | ARG | A | 177 | 34.625 | 22.712 | 15.267 | 1.00 | 29.88 | C |
| ATOM | 1313 | CD  | ARG | A | 177 | 34.653 | 23.460 | 13.973 | 1.00 | 32.39 | C |
| ATOM | 1314 | NE  | ARG | A | 177 | 33.683 | 22.854 | 13.084 | 1.00 | 34.54 | N |
| ATOM | 1315 | CZ  | ARG | A | 177 | 33.841 | 22.701 | 11.790 | 1.00 | 37.31 | C |
| ATOM | 1316 | NH1 | ARG | A | 177 | 34.952 | 23.110 | 11.189 | 1.00 | 38.34 | N |
| ATOM | 1317 | NH2 | ARG | A | 177 | 32.877 | 22.126 | 11.088 | 1.00 | 38.88 | N |
| ATOM | 1318 | N   | GLY | A | 178 | 38.950 | 21.510 | 16.743 | 1.00 | 26.35 | N |
| ATOM | 1319 | CA  | GLY | A | 178 | 39.998 | 21.470 | 17.753 | 1.00 | 25.46 | C |
| ATOM | 1320 | C   | GLY | A | 178 | 39.473 | 21.514 | 19.176 | 1.00 | 25.27 | C |
| ATOM | 1321 | O   | GLY | A | 178 | 40.213 | 21.818 | 20.123 | 1.00 | 25.46 | O |
| ATOM | 1322 | N   | TRP | A | 179 | 38.199 | 21.202 | 19.359 | 1.00 | 24.30 | N |
| ATOM | 1323 | CA  | TRP | A | 179 | 37.639 | 21.260 | 20.692 | 1.00 | 24.02 | C |
| ATOM | 1324 | C   | TRP | A | 179 | 38.290 | 20.266 | 21.638 | 1.00 | 23.85 | C |
| ATOM | 1325 | O   | TRP | A | 179 | 38.958 | 19.333 | 21.226 | 1.00 | 22.62 | O |
| ATOM | 1326 | CB  | TRP | A | 179 | 36.136 | 21.011 | 20.674 | 1.00 | 23.73 | C |
| ATOM | 1327 | CG  | TRP | A | 179 | 35.346 | 22.061 | 19.962 | 1.00 | 23.92 | C |
| ATOM | 1328 | CD1 | TRP | A | 179 | 35.787 | 23.291 | 19.531 | 1.00 | 22.69 | C |
| ATOM | 1329 | CD2 | TRP | A | 179 | 33.968 | 21.981 | 19.594 | 1.00 | 23.74 | C |
| ATOM | 1330 | NE1 | TRP | A | 179 | 34.765 | 23.968 | 18.912 | 1.00 | 24.45 | N |
| ATOM | 1331 | CE2 | TRP | A | 179 | 33.636 | 23.183 | 18.929 | 1.00 | 24.47 | C |
| ATOM | 1332 | CE3 | TRP | A | 179 | 32.984 | 21.002 | 19.730 | 1.00 | 23.10 | C |
| ATOM | 1333 | CZ2 | TRP | A | 179 | 32.379 | 23.422 | 18.414 | 1.00 | 23.69 | C |
| ATOM | 1334 | CZ3 | TRP | A | 179 | 31.733 | 21.241 | 19.211 | 1.00 | 21.89 | C |
| ATOM | 1335 | CH2 | TRP | A | 179 | 31.435 | 22.445 | 18.573 | 1.00 | 23.90 | C |
| ATOM | 1336 | N   | GLY | A | 180 | 38.080 | 20.499 | 22.925 | 1.00 | 24.08 | N |
| ATOM | 1337 | CA  | GLY | A | 180 | 38.488 | 19.558 | 23.941 | 1.00 | 24.08 | C |
| ATOM | 1338 | C   | GLY | A | 180 | 37.437 | 18.476 | 24.103 | 1.00 | 24.64 | C |
| ATOM | 1339 | O   | GLY | A | 180 | 36.618 | 18.234 | 23.202 | 1.00 | 24.66 | O |
| ATOM | 1340 | N   | GLN | A | 181 | 37.437 | 17.830 | 25.261 | 1.00 | 24.77 | N |
| ATOM | 1341 | CA  | GLN | A | 181 | 36.575 | 16.682 | 25.471 | 1.00 | 25.23 | C |
| ATOM | 1342 | C   | GLN | A | 181 | 35.117 | 17.039 | 25.725 | 1.00 | 24.50 | C |
| ATOM | 1343 | O   | GLN | A | 181 | 34.779 | 18.151 | 26.149 | 1.00 | 24.42 | O |
| ATOM | 1344 | CB  | GLN | A | 181 | 37.094 | 15.847 | 26.646 | 1.00 | 25.76 | C |
| ATOM | 1345 | CG  | GLN | A | 181 | 36.720 | 16.409 | 28.025 | 1.00 | 28.85 | C |
| ATOM | 1346 | CD  | GLN | A | 181 | 37.046 | 15.434 | 29.156 | 1.00 | 33.38 | C |
| ATOM | 1347 | OE1 | GLN | A | 181 | 38.186 | 15.003 | 29.293 | 1.00 | 36.10 | O |
| ATOM | 1348 | NE2 | GLN | A | 181 | 36.044 | 15.085 | 29.958 | 1.00 | 36.04 | N |
| ATOM | 1349 | N   | LEU | A | 182 | 34.262 | 16.078 | 25.423 | 1.00 | 23.71 | N |
| ATOM | 1350 | CA  | LEU | A | 182 | 32.857 | 16.110 | 25.792 | 1.00 | 23.70 | C |
| ATOM | 1351 | C   | LEU | A | 182 | 32.876 | 16.040 | 27.317 | 1.00 | 22.68 | C |
| ATOM | 1352 | O   | LEU | A | 182 | 33.406 | 15.079 | 27.849 | 1.00 | 21.72 | O |
| ATOM | 1353 | CB  | LEU | A | 182 | 32.179 | 14.836 | 25.273 | 1.00 | 23.82 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1354 | CG  | LEU | A | 182 | 30.661 | 14.693 | 25.199 | 1.00 | 26.38 | C |
| ATOM | 1355 | CD1 | LEU | A | 182 | 30.243 | 13.231 | 25.368 | 1.00 | 26.04 | C |
| ATOM | 1356 | CD2 | LEU | A | 182 | 29.977 | 15.501 | 26.192 | 1.00 | 29.73 | C |
| ATOM | 1357 | N   | THR | A | 183 | 32.323 | 17.031 | 28.021 | 1.00 | 21.93 | N |
| ATOM | 1358 | CA  | THR | A | 183 | 32.300 | 16.971 | 29.484 | 1.00 | 21.44 | C |
| ATOM | 1359 | C   | THR | A | 183 | 31.004 | 16.388 | 29.984 | 1.00 | 21.27 | C |
| ATOM | 1360 | O   | THR | A | 183 | 30.972 | 15.766 | 31.032 | 1.00 | 21.29 | O |
| ATOM | 1361 | CB  | THR | A | 183 | 32.490 | 18.362 | 30.150 | 1.00 | 21.73 | C |
| ATOM | 1362 | OG1 | THR | A | 183 | 31.463 | 19.257 | 29.715 | 1.00 | 20.35 | O |
| ATOM | 1363 | CG2 | THR | A | 183 | 33.796 | 19.015 | 29.725 | 1.00 | 20.91 | C |
| ATOM | 1364 | N   | SER | A | 184 | 29.918 | 16.590 | 29.251 | 1.00 | 21.42 | N |
| ATOM | 1365 | CA  | SER | A | 184 | 28.649 | 16.053 | 29.689 | 1.00 | 21.45 | C |
| ATOM | 1366 | C   | SER | A | 184 | 27.537 | 16.272 | 28.714 | 1.00 | 21.46 | C |
| ATOM | 1367 | O   | SER | A | 184 | 27.672 | 17.031 | 27.753 | 1.00 | 21.17 | O |
| ATOM | 1368 | CB  | SER | A | 184 | 28.243 | 16.687 | 31.006 | 1.00 | 21.74 | C |
| ATOM | 1369 | OG  | SER | A | 184 | 27.919 | 18.049 | 30.845 | 1.00 | 23.24 | O |
| ATOM | 1370 | N   | ASN | A | 185 | 26.445 | 15.575 | 28.982 | 1.00 | 21.21 | N |
| ATOM | 1371 | CA  | ASN | A | 185 | 25.216 | 15.712 | 28.245 | 1.00 | 22.29 | C |
| ATOM | 1372 | C   | ASN | A | 185 | 24.154 | 16.005 | 29.273 | 1.00 | 22.08 | C |
| ATOM | 1373 | O   | ASN | A | 185 | 23.886 | 15.184 | 30.135 | 1.00 | 22.25 | O |
| ATOM | 1374 | CB  | ASN | A | 185 | 24.856 | 14.416 | 27.497 | 1.00 | 22.67 | C |
| ATOM | 1375 | CG  | ASN | A | 185 | 25.885 | 14.037 | 26.454 | 1.00 | 23.57 | C |
| ATOM | 1376 | OD1 | ASN | A | 185 | 26.646 | 13.097 | 26.655 | 1.00 | 27.51 | O |
| ATOM | 1377 | ND2 | ASN | A | 185 | 25.905 | 14.754 | 25.329 | 1.00 | 24.27 | N |
| ATOM | 1378 | N   | LEU | A | 186 | 23.574 | 17.189 | 29.202 | 1.00 | 22.01 | N |
| ATOM | 1379 | CA  | LEU | A | 186 | 22.529 | 17.563 | 30.135 | 1.00 | 22.03 | C |
| ATOM | 1380 | C   | LEU | A | 186 | 21.170 | 17.219 | 29.558 | 1.00 | 22.00 | C |
| ATOM | 1381 | O   | LEU | A | 186 | 20.844 | 17.592 | 28.435 | 1.00 | 22.34 | O |
| ATOM | 1382 | CB  | LEU | A | 186 | 22.578 | 19.065 | 30.423 | 1.00 | 21.68 | C |
| ATOM | 1383 | CG  | LEU | A | 186 | 21.707 | 19.538 | 31.588 | 1.00 | 22.25 | C |
| ATOM | 1384 | CD1 | LEU | A | 186 | 22.252 | 18.985 | 32.891 | 1.00 | 22.43 | C |
| ATOM | 1385 | CD2 | LEU | A | 186 | 21.643 | 21.098 | 31.648 | 1.00 | 23.35 | C |
| ATOM | 1386 | N   | LEU | A | 187 | 20.377 | 16.518 | 30.344 | 1.00 | 22.19 | N |
| ATOM | 1387 | CA  | LEU | A | 187 | 19.009 | 16.198 | 29.979 | 1.00 | 21.95 | C |
| ATOM | 1388 | C   | LEU | A | 187 | 18.149 | 17.286 | 30.603 | 1.00 | 21.91 | C |
| ATOM | 1389 | O   | LEU | A | 187 | 18.232 | 17.521 | 31.823 | 1.00 | 21.61 | O |
| ATOM | 1390 | CB  | LEU | A | 187 | 18.616 | 14.830 | 30.527 | 1.00 | 21.55 | C |
| ATOM | 1391 | CG  | LEU | A | 187 | 17.129 | 14.488 | 30.477 | 1.00 | 22.78 | C |
| ATOM | 1392 | CD1 | LEU | A | 187 | 16.616 | 14.429 | 29.054 | 1.00 | 23.66 | C |
| ATOM | 1393 | CD2 | LEU | A | 187 | 16.866 | 13.143 | 31.174 | 1.00 | 22.84 | C |
| ATOM | 1394 | N   | LEU | A | 188 | 17.348 | 17.956 | 29.770 | 1.00 | 21.56 | N |
| ATOM | 1395 | CA  | LEU | A | 188 | 16.461 | 19.000 | 30.227 | 1.00 | 22.26 | C |
| ATOM | 1396 | C   | LEU | A | 188 | 14.993 | 18.662 | 29.920 | 1.00 | 22.55 | C |
| ATOM | 1397 | O   | LEU | A | 188 | 14.588 | 18.517 | 28.760 | 1.00 | 23.16 | O |
| ATOM | 1398 | CB  | LEU | A | 188 | 16.827 | 20.327 | 29.562 | 1.00 | 22.84 | C |
| ATOM | 1399 | CG  | LEU | A | 188 | 18.244 | 20.840 | 29.821 | 1.00 | 22.60 | C |
| ATOM | 1400 | CD1 | LEU | A | 188 | 18.967 | 21.111 | 28.523 | 1.00 | 23.92 | C |
| ATOM | 1401 | CD2 | LEU | A | 188 | 18.177 | 22.088 | 30.655 | 1.00 | 24.56 | C |
| ATOM | 1402 | N   | ILE | A | 189 | 14.181 | 18.577 | 30.958 | 1.00 | 22.15 | N |
| ATOM | 1403 | CA  | ILE | A | 189 | 12.769 | 18.315 | 30.756 | 1.00 | 22.34 | C |
| ATOM | 1404 | C   | ILE | A | 189 | 11.996 | 19.395 | 31.460 | 1.00 | 22.37 | C |
| ATOM | 1405 | O   | ILE | A | 189 | 12.072 | 19.528 | 32.692 | 1.00 | 22.77 | O |
| ATOM | 1406 | CB  | ILE | A | 189 | 12.377 | 16.953 | 31.281 | 1.00 | 21.60 | C |
| ATOM | 1407 | CG1 | ILE | A | 189 | 13.254 | 15.888 | 30.638 | 1.00 | 21.85 | C |
| ATOM | 1408 | CG2 | ILE | A | 189 | 10.928 | 16.708 | 30.958 | 1.00 | 22.51 | C |
| ATOM | 1409 | CD1 | ILE | A | 189 | 12.918 | 14.425 | 31.075 | 1.00 | 23.06 | C |
| ATOM | 1410 | N   | GLY | A | 190 | 11.276 | 20.186 | 30.673 | 1.00 | 22.37 | N |
| ATOM | 1411 | CA  | GLY | A | 190 | 10.587 | 21.336 | 31.206 | 1.00 | 22.29 | C |
| ATOM | 1412 | C   | GLY | A | 190 | 9.124  | 21.342 | 30.902 | 1.00 | 22.48 | C |
| ATOM | 1413 | O   | GLY | A | 190 | 8.652  | 20.633 | 30.007 | 1.00 | 22.39 | O |
| ATOM | 1414 | N   | MET | A | 191 | 8.402  | 22.134 | 31.687 | 1.00 | 22.74 | N |

|      |      |     |           |        |        |        |      |       |   |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 1415 | CA  | MET A 191 | 6.991  | 22.339 | 31.467 | 1.00 | 23.16 | C |
| ATOM | 1416 | C   | MET A 191 | 6.838  | 23.482 | 30.478 | 1.00 | 22.94 | C |
| ATOM | 1417 | O   | MET A 191 | 7.738  | 24.329 | 30.338 | 1.00 | 23.03 | O |
| ATOM | 1418 | CB  | MET A 191 | 6.283  | 22.673 | 32.784 | 1.00 | 23.69 | C |
| ATOM | 1419 | CG  | MET A 191 | 6.224  | 21.513 | 33.741 | 1.00 | 25.02 | C |
| ATOM | 1420 | SD  | MET A 191 | 5.664  | 21.927 | 35.415 | 1.00 | 28.11 | S |
| ATOM | 1421 | CE  | MET A 191 | 4.016  | 22.460 | 35.097 | 1.00 | 28.35 | C |
| ATOM | 1422 | N   | GLU A 192 | 5.712  | 23.492 | 29.773 | 1.00 | 22.60 | N |
| ATOM | 1423 | CA  | GLU A 192 | 5.410  | 24.544 | 28.810 | 1.00 | 22.83 | C |
| ATOM | 1424 | C   | GLU A 192 | 5.495  | 25.895 | 29.490 | 1.00 | 22.51 | C |
| ATOM | 1425 | O   | GLU A 192 | 5.062  | 26.046 | 30.614 | 1.00 | 22.41 | O |
| ATOM | 1426 | CB  | GLU A 192 | 4.005  | 24.342 | 28.249 | 1.00 | 22.86 | C |
| ATOM | 1427 | CG  | GLU A 192 | 2.925  | 24.367 | 29.315 | 1.00 | 24.36 | C |
| ATOM | 1428 | CD  | GLU A 192 | 1.572  | 23.891 | 28.814 | 1.00 | 25.71 | C |
| ATOM | 1429 | OE1 | GLU A 192 | 1.503  | 23.294 | 27.718 | 1.00 | 25.51 | O |
| ATOM | 1430 | OE2 | GLU A 192 | 0.582  | 24.128 | 29.525 | 1.00 | 26.30 | O |
| ATOM | 1431 | N   | GLY A 193 | 6.069  | 26.888 | 28.828 | 1.00 | 22.95 | N |
| ATOM | 1432 | CA  | GLY A 193 | 6.185  | 28.199 | 29.444 | 1.00 | 22.50 | C |
| ATOM | 1433 | C   | GLY A 193 | 7.465  | 28.414 | 30.254 | 1.00 | 22.36 | C |
| ATOM | 1434 | O   | GLY A 193 | 7.756  | 29.544 | 30.602 | 1.00 | 23.08 | O |
| ATOM | 1435 | N   | ASN A 194 | 8.219  | 27.361 | 30.566 | 1.00 | 21.60 | N |
| ATOM | 1436 | CA  | ASN A 194 | 9.456  | 27.506 | 31.341 | 1.00 | 21.44 | C |
| ATOM | 1437 | C   | ASN A 194 | 10.489 | 28.320 | 30.581 | 1.00 | 21.19 | C |
| ATOM | 1438 | O   | ASN A 194 | 10.635 | 28.134 | 29.372 | 1.00 | 22.08 | O |
| ATOM | 1439 | CB  | ASN A 194 | 10.099 | 26.147 | 31.629 | 1.00 | 21.05 | C |
| ATOM | 1440 | CG  | ASN A 194 | 9.494  | 25.435 | 32.801 | 1.00 | 20.86 | C |
| ATOM | 1441 | OD1 | ASN A 194 | 8.509  | 25.883 | 33.385 | 1.00 | 22.48 | O |
| ATOM | 1442 | ND2 | ASN A 194 | 10.092 | 24.312 | 33.167 | 1.00 | 17.74 | N |
| ATOM | 1443 | N   | VAL A 195 | 11.213 | 29.183 | 31.290 | 1.00 | 20.69 | N |
| ATOM | 1444 | CA  | VAL A 195 | 12.268 | 29.993 | 30.701 | 1.00 | 20.84 | C |
| ATOM | 1445 | C   | VAL A 195 | 13.572 | 29.854 | 31.450 | 1.00 | 20.06 | C |
| ATOM | 1446 | O   | VAL A 195 | 13.601 | 29.874 | 32.681 | 1.00 | 20.75 | O |
| ATOM | 1447 | CB  | VAL A 195 | 11.903 | 31.502 | 30.686 | 1.00 | 21.41 | C |
| ATOM | 1448 | CG1 | VAL A 195 | 13.081 | 32.357 | 30.219 | 1.00 | 22.24 | C |
| ATOM | 1449 | CG2 | VAL A 195 | 10.666 | 31.767 | 29.843 | 1.00 | 22.30 | C |
| ATOM | 1450 | N   | THR A 196 | 14.651 | 29.673 | 30.702 | 1.00 | 19.51 | N |
| ATOM | 1451 | CA  | THR A 196 | 15.993 | 29.737 | 31.257 | 1.00 | 19.52 | C |
| ATOM | 1452 | C   | THR A 196 | 16.487 | 31.117 | 30.820 | 1.00 | 19.98 | C |
| ATOM | 1453 | O   | THR A 196 | 16.653 | 31.352 | 29.620 | 1.00 | 19.56 | O |
| ATOM | 1454 | CB  | THR A 196 | 16.896 | 28.677 | 30.675 | 1.00 | 19.26 | C |
| ATOM | 1455 | OG1 | THR A 196 | 16.526 | 27.366 | 31.162 | 1.00 | 21.13 | O |
| ATOM | 1456 | CG2 | THR A 196 | 18.309 | 28.886 | 31.185 | 1.00 | 19.85 | C |
| ATOM | 1457 | N   | PRO A 197 | 16.627 | 32.043 | 31.767 | 1.00 | 20.27 | N |
| ATOM | 1458 | CA  | PRO A 197 | 17.046 | 33.412 | 31.463 | 1.00 | 20.52 | C |
| ATOM | 1459 | C   | PRO A 197 | 18.431 | 33.497 | 30.836 | 1.00 | 20.89 | C |
| ATOM | 1460 | O   | PRO A 197 | 19.277 | 32.609 | 31.025 | 1.00 | 20.66 | O |
| ATOM | 1461 | CB  | PRO A 197 | 17.018 | 34.099 | 32.825 | 1.00 | 21.22 | C |
| ATOM | 1462 | CG  | PRO A 197 | 16.144 | 33.263 | 33.657 | 1.00 | 21.01 | C |
| ATOM | 1463 | CD  | PRO A 197 | 16.309 | 31.872 | 33.189 | 1.00 | 20.28 | C |
| ATOM | 1464 | N   | ALA A 198 | 18.633 | 34.577 | 30.089 | 1.00 | 20.28 | N |
| ATOM | 1465 | CA  | ALA A 198 | 19.841 | 34.817 | 29.341 | 1.00 | 20.22 | C |
| ATOM | 1466 | C   | ALA A 198 | 21.130 | 34.634 | 30.146 | 1.00 | 20.58 | C |
| ATOM | 1467 | O   | ALA A 198 | 21.284 | 35.186 | 31.235 | 1.00 | 19.91 | O |
| ATOM | 1468 | CB  | ALA A 198 | 19.791 | 36.222 | 28.759 | 1.00 | 20.52 | C |
| ATOM | 1469 | N   | HIS A 199 | 22.062 | 33.891 | 29.563 | 1.00 | 20.87 | N |
| ATOM | 1470 | CA  | HIS A 199 | 23.371 | 33.646 | 30.158 | 1.00 | 21.41 | C |
| ATOM | 1471 | C   | HIS A 199 | 24.281 | 33.168 | 29.063 | 1.00 | 21.82 | C |
| ATOM | 1472 | O   | HIS A 199 | 23.826 | 32.892 | 27.943 | 1.00 | 21.80 | O |
| ATOM | 1473 | CB  | HIS A 199 | 23.305 | 32.534 | 31.198 | 1.00 | 21.44 | C |
| ATOM | 1474 | CG  | HIS A 199 | 22.915 | 31.220 | 30.617 | 1.00 | 22.21 | C |
| ATOM | 1475 | ND1 | HIS A 199 | 21.619 | 30.940 | 30.253 | 1.00 | 21.93 | N |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1476 | CD2 | HIS | A | 199 | 23.644 | 30.120 | 30.296 | 1.00 | 22.04 | C |
| ATOM | 1477 | CE1 | HIS | A | 199 | 21.561 | 29.721 | 29.749 | 1.00 | 23.76 | C |
| ATOM | 1478 | NE2 | HIS | A | 199 | 22.777 | 29.214 | 29.737 | 1.00 | 22.57 | N |
| ATOM | 1479 | N   | TYR | A | 200 | 25.568 | 33.060 | 29.384 | 1.00 | 22.40 | N |
| ATOM | 1480 | CA  | TYR | A | 200 | 26.536 | 32.456 | 28.469 | 1.00 | 22.34 | C |
| ATOM | 1481 | C   | TYR | A | 200 | 27.225 | 31.316 | 29.197 | 1.00 | 22.03 | C |
| ATOM | 1482 | O   | TYR | A | 200 | 27.328 | 31.330 | 30.425 | 1.00 | 21.90 | O |
| ATOM | 1483 | CB  | TYR | A | 200 | 27.544 | 33.458 | 27.924 | 1.00 | 22.22 | C |
| ATOM | 1484 | CG  | TYR | A | 200 | 28.517 | 34.051 | 28.924 | 1.00 | 22.16 | C |
| ATOM | 1485 | CD1 | TYR | A | 200 | 29.746 | 33.454 | 29.171 | 1.00 | 21.36 | C |
| ATOM | 1486 | CD2 | TYR | A | 200 | 28.236 | 35.246 | 29.565 | 1.00 | 22.58 | C |
| ATOM | 1487 | CE1 | TYR | A | 200 | 30.638 | 33.997 | 30.052 | 1.00 | 21.48 | C |
| ATOM | 1488 | CE2 | TYR | A | 200 | 29.128 | 35.806 | 30.462 | 1.00 | 21.46 | C |
| ATOM | 1489 | CZ  | TYR | A | 200 | 30.334 | 35.189 | 30.695 | 1.00 | 22.03 | C |
| ATOM | 1490 | OH  | TYR | A | 200 | 31.230 | 35.733 | 31.593 | 1.00 | 20.69 | O |
| ATOM | 1491 | N   | ASP | A | 201 | 27.681 | 30.310 | 28.444 | 1.00 | 22.42 | N |
| ATOM | 1492 | CA  | ASP | A | 201 | 28.381 | 29.152 | 29.048 | 1.00 | 22.10 | C |
| ATOM | 1493 | C   | ASP | A | 201 | 29.801 | 29.142 | 28.531 | 1.00 | 21.96 | C |
| ATOM | 1494 | O   | ASP | A | 201 | 30.018 | 29.601 | 27.433 | 1.00 | 22.26 | O |
| ATOM | 1495 | CB  | ASP | A | 201 | 27.722 | 27.840 | 28.661 | 1.00 | 21.97 | C |
| ATOM | 1496 | CG  | ASP | A | 201 | 26.311 | 27.714 | 29.181 | 1.00 | 21.99 | C |
| ATOM | 1497 | OD1 | ASP | A | 201 | 26.126 | 27.649 | 30.421 | 1.00 | 22.61 | O |
| ATOM | 1498 | OD2 | ASP | A | 201 | 25.330 | 27.624 | 28.412 | 1.00 | 19.35 | O |
| ATOM | 1499 | N   | GLU | A | 202 | 30.769 | 28.620 | 29.283 | 1.00 | 21.66 | N |
| ATOM | 1500 | CA  | GLU | A | 202 | 32.146 | 28.612 | 28.773 | 1.00 | 23.16 | C |
| ATOM | 1501 | C   | GLU | A | 202 | 32.515 | 27.334 | 28.035 | 1.00 | 23.38 | C |
| ATOM | 1502 | O   | GLU | A | 202 | 33.684 | 26.951 | 28.049 | 1.00 | 25.48 | O |
| ATOM | 1503 | CB  | GLU | A | 202 | 33.178 | 28.774 | 29.897 | 1.00 | 23.46 | C |
| ATOM | 1504 | CG  | GLU | A | 202 | 33.110 | 30.064 | 30.681 | 1.00 | 26.52 | C |
| ATOM | 1505 | CD  | GLU | A | 202 | 34.233 | 30.132 | 31.704 | 1.00 | 28.11 | C |
| ATOM | 1506 | OE1 | GLU | A | 202 | 34.207 | 29.387 | 32.698 | 1.00 | 29.06 | O |
| ATOM | 1507 | OE2 | GLU | A | 202 | 35.148 | 30.920 | 31.490 | 1.00 | 31.04 | O |
| ATOM | 1508 | N   | GLN | A | 203 | 31.538 | 26.632 | 27.476 | 1.00 | 22.70 | N |
| ATOM | 1509 | CA  | GLN | A | 203 | 31.808 | 25.451 | 26.685 | 1.00 | 22.01 | C |
| ATOM | 1510 | C   | GLN | A | 203 | 31.049 | 25.576 | 25.373 | 1.00 | 21.93 | C |
| ATOM | 1511 | O   | GLN | A | 203 | 30.113 | 26.378 | 25.253 | 1.00 | 22.49 | O |
| ATOM | 1512 | CB  | GLN | A | 203 | 31.409 | 24.169 | 27.427 | 1.00 | 22.02 | C |
| ATOM | 1513 | CG  | GLN | A | 203 | 32.287 | 23.822 | 28.657 | 1.00 | 22.33 | C |
| ATOM | 1514 | CD  | GLN | A | 203 | 32.103 | 22.379 | 29.165 | 1.00 | 23.14 | C |
| ATOM | 1515 | OE1 | GLN | A | 203 | 31.948 | 21.448 | 28.370 | 1.00 | 21.46 | O |
| ATOM | 1516 | NE2 | GLN | A | 203 | 32.138 | 22.203 | 30.489 | 1.00 | 21.21 | N |
| ATOM | 1517 | N   | GLN | A | 204 | 31.486 | 24.807 | 24.380 | 1.00 | 21.81 | N |
| ATOM | 1518 | CA  | GLN | A | 204 | 30.806 | 24.720 | 23.092 | 1.00 | 21.45 | C |
| ATOM | 1519 | C   | GLN | A | 204 | 29.610 | 23.799 | 23.295 | 1.00 | 21.12 | C |
| ATOM | 1520 | O   | GLN | A | 204 | 29.673 | 22.862 | 24.088 | 1.00 | 20.29 | O |
| ATOM | 1521 | CB  | GLN | A | 204 | 31.740 | 24.140 | 22.040 | 1.00 | 21.75 | C |
| ATOM | 1522 | CG  | GLN | A | 204 | 33.033 | 24.928 | 21.852 | 1.00 | 21.56 | C |
| ATOM | 1523 | CD  | GLN | A | 204 | 32.856 | 26.198 | 21.000 | 1.00 | 21.57 | C |
| ATOM | 1524 | OE1 | GLN | A | 204 | 31.741 | 26.609 | 20.692 | 1.00 | 20.30 | O |
| ATOM | 1525 | NE2 | GLN | A | 204 | 33.966 | 26.776 | 20.594 | 1.00 | 18.60 | N |
| ATOM | 1526 | N   | ASN | A | 205 | 28.522 | 24.060 | 22.580 | 1.00 | 21.25 | N |
| ATOM | 1527 | CA  | ASN | A | 205 | 27.291 | 23.316 | 22.795 | 1.00 | 21.04 | C |
| ATOM | 1528 | C   | ASN | A | 205 | 26.529 | 22.977 | 21.526 | 1.00 | 21.25 | C |
| ATOM | 1529 | O   | ASN | A | 205 | 26.160 | 23.880 | 20.747 | 1.00 | 20.22 | O |
| ATOM | 1530 | CB  | ASN | A | 205 | 26.387 | 24.194 | 23.654 | 1.00 | 21.95 | C |
| ATOM | 1531 | CG  | ASN | A | 205 | 25.116 | 23.507 | 24.098 | 1.00 | 21.98 | C |
| ATOM | 1532 | OD1 | ASN | A | 205 | 24.759 | 22.418 | 23.643 | 1.00 | 21.21 | O |
| ATOM | 1533 | ND2 | ASN | A | 205 | 24.400 | 24.178 | 24.979 | 1.00 | 17.72 | N |
| ATOM | 1534 | N   | PHE | A | 206 | 26.314 | 21.677 | 21.319 | 1.00 | 19.90 | N |
| ATOM | 1535 | CA  | PHE | A | 206 | 25.339 | 21.230 | 20.354 | 1.00 | 19.77 | C |
| ATOM | 1536 | C   | PHE | A | 206 | 24.085 | 20.869 | 21.150 | 1.00 | 19.25 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1537 | O   | PHE | A | 206 | 24.094 | 19.939 | 21.959 | 1.00 | 19.15 | O |
| ATOM | 1538 | CB  | PHE | A | 206 | 25.849 | 20.049 | 19.545 | 1.00 | 20.09 | C |
| ATOM | 1539 | CG  | PHE | A | 206 | 26.786 | 20.442 | 18.454 | 1.00 | 19.77 | C |
| ATOM | 1540 | CD1 | PHE | A | 206 | 26.371 | 21.294 | 17.453 | 1.00 | 22.21 | C |
| ATOM | 1541 | CD2 | PHE | A | 206 | 28.079 | 19.973 | 18.435 | 1.00 | 20.21 | C |
| ATOM | 1542 | CE1 | PHE | A | 206 | 27.213 | 21.643 | 16.434 | 1.00 | 22.06 | C |
| ATOM | 1543 | CE2 | PHE | A | 206 | 28.941 | 20.336 | 17.418 | 1.00 | 20.66 | C |
| ATOM | 1544 | CZ  | PHE | A | 206 | 28.504 | 21.190 | 16.427 | 1.00 | 22.18 | C |
| ATOM | 1545 | N   | PHE | A | 207 | 23.009 | 21.596 | 20.869 | 1.00 | 18.42 | N |
| ATOM | 1546 | CA  | PHE | A | 207 | 21.760 | 21.590 | 21.620 | 1.00 | 18.78 | C |
| ATOM | 1547 | C   | PHE | A | 207 | 20.732 | 20.841 | 20.804 | 1.00 | 19.36 | C |
| ATOM | 1548 | O   | PHE | A | 207 | 20.241 | 21.359 | 19.818 | 1.00 | 19.26 | O |
| ATOM | 1549 | CB  | PHE | A | 207 | 21.366 | 23.063 | 21.836 | 1.00 | 18.70 | C |
| ATOM | 1550 | CG  | PHE | A | 207 | 20.120 | 23.301 | 22.635 | 1.00 | 17.94 | C |
| ATOM | 1551 | CD1 | PHE | A | 207 | 18.899 | 23.404 | 22.007 | 1.00 | 17.78 | C |
| ATOM | 1552 | CD2 | PHE | A | 207 | 20.188 | 23.548 | 23.989 | 1.00 | 18.50 | C |
| ATOM | 1553 | CE1 | PHE | A | 207 | 17.772 | 23.684 | 22.713 | 1.00 | 19.52 | C |
| ATOM | 1554 | CE2 | PHE | A | 207 | 19.052 | 23.823 | 24.705 | 1.00 | 20.66 | C |
| ATOM | 1555 | CZ  | PHE | A | 207 | 17.836 | 23.909 | 24.053 | 1.00 | 19.44 | C |
| ATOM | 1556 | N   | ALA | A | 208 | 20.435 | 19.618 | 21.234 | 1.00 | 19.90 | N |
| ATOM | 1557 | CA  | ALA | A | 208 | 19.628 | 18.670 | 20.469 | 1.00 | 20.17 | C |
| ATOM | 1558 | C   | ALA | A | 208 | 18.210 | 18.541 | 20.991 | 1.00 | 20.52 | C |
| ATOM | 1559 | O   | ALA | A | 208 | 17.971 | 17.946 | 22.047 | 1.00 | 20.61 | O |
| ATOM | 1560 | CB  | ALA | A | 208 | 20.294 | 17.308 | 20.494 | 1.00 | 19.33 | C |
| ATOM | 1561 | N   | GLN | A | 209 | 17.270 | 19.076 | 20.219 | 1.00 | 20.94 | N |
| ATOM | 1562 | CA  | GLN | A | 209 | 15.880 | 19.062 | 20.627 | 1.00 | 20.82 | C |
| ATOM | 1563 | C   | GLN | A | 209 | 15.227 | 17.712 | 20.323 | 1.00 | 20.75 | C |
| ATOM | 1564 | O   | GLN | A | 209 | 15.401 | 17.129 | 19.224 | 1.00 | 19.59 | O |
| ATOM | 1565 | CB  | GLN | A | 209 | 15.141 | 20.216 | 19.961 | 1.00 | 20.91 | C |
| ATOM | 1566 | CG  | GLN | A | 209 | 13.735 | 20.431 | 20.463 | 1.00 | 20.52 | C |
| ATOM | 1567 | CD  | GLN | A | 209 | 13.673 | 20.840 | 21.928 | 1.00 | 20.69 | C |
| ATOM | 1568 | OE1 | GLN | A | 209 | 14.702 | 21.155 | 22.562 | 1.00 | 19.72 | O |
| ATOM | 1569 | NE2 | GLN | A | 209 | 12.460 | 20.852 | 22.473 | 1.00 | 19.21 | N |
| ATOM | 1570 | N   | ILE | A | 210 | 14.442 | 17.248 | 21.296 | 1.00 | 20.72 | N |
| ATOM | 1571 | CA  | ILE | A | 210 | 13.853 | 15.922 | 21.252 | 1.00 | 21.43 | C |
| ATOM | 1572 | C   | ILE | A | 210 | 12.334 | 15.911 | 21.292 | 1.00 | 21.72 | C |
| ATOM | 1573 | O   | ILE | A | 210 | 11.728 | 15.195 | 20.534 | 1.00 | 22.12 | O |
| ATOM | 1574 | CB  | ILE | A | 210 | 14.396 | 15.095 | 22.424 | 1.00 | 21.84 | C |
| ATOM | 1575 | CG1 | ILE | A | 210 | 15.859 | 14.733 | 22.156 | 1.00 | 22.48 | C |
| ATOM | 1576 | CG2 | ILE | A | 210 | 13.581 | 13.832 | 22.622 | 1.00 | 21.83 | C |
| ATOM | 1577 | CD1 | ILE | A | 210 | 16.631 | 14.354 | 23.382 | 1.00 | 24.34 | C |
| ATOM | 1578 | N   | LYS | A | 211 | 11.728 | 16.677 | 22.188 | 1.00 | 22.08 | N |
| ATOM | 1579 | CA  | LYS | A | 211 | 10.279 | 16.715 | 22.319 | 1.00 | 21.72 | C |
| ATOM | 1580 | C   | LYS | A | 211 | 9.858  | 18.130 | 22.564 | 1.00 | 21.67 | C |
| ATOM | 1581 | O   | LYS | A | 211 | 10.468 | 18.841 | 23.372 | 1.00 | 20.87 | O |
| ATOM | 1582 | CB  | LYS | A | 211 | 9.797  | 15.856 | 23.487 | 1.00 | 22.44 | C |
| ATOM | 1583 | CG  | LYS | A | 211 | 8.267  | 15.562 | 23.479 | 1.00 | 23.29 | C |
| ATOM | 1584 | CD  | LYS | A | 211 | 7.791  | 15.022 | 24.824 | 1.00 | 25.02 | C |
| ATOM | 1585 | CE  | LYS | A | 211 | 6.494  | 14.215 | 24.757 | 1.00 | 26.00 | C |
| ATOM | 1586 | NZ  | LYS | A | 211 | 5.561  | 14.522 | 23.634 | 1.00 | 26.43 | N |
| ATOM | 1587 | N   | GLY | A | 212 | 8.798  | 18.541 | 21.875 | 1.00 | 21.35 | N |
| ATOM | 1588 | CA  | GLY | A | 212 | 8.306  | 19.891 | 21.994 | 1.00 | 21.71 | C |
| ATOM | 1589 | C   | GLY | A | 212 | 9.195  | 20.906 | 21.297 | 1.00 | 21.63 | C |
| ATOM | 1590 | O   | GLY | A | 212 | 10.150 | 20.572 | 20.591 | 1.00 | 21.32 | O |
| ATOM | 1591 | N   | TYR | A | 213 | 8.871  | 22.166 | 21.522 | 1.00 | 22.35 | N |
| ATOM | 1592 | CA  | TYR | A | 213 | 9.533  | 23.279 | 20.862 | 1.00 | 22.42 | C |
| ATOM | 1593 | C   | TYR | A | 213 | 10.028 | 24.293 | 21.868 | 1.00 | 22.33 | C |
| ATOM | 1594 | O   | TYR | A | 213 | 9.340  | 24.589 | 22.853 | 1.00 | 21.55 | O |
| ATOM | 1595 | CB  | TYR | A | 213 | 8.556  | 23.951 | 19.916 | 1.00 | 23.46 | C |
| ATOM | 1596 | CG  | TYR | A | 213 | 8.114  | 23.034 | 18.815 | 1.00 | 24.81 | C |
| ATOM | 1597 | CD1 | TYR | A | 213 | 7.100  | 22.112 | 19.020 | 1.00 | 28.16 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1598 | CD2 | TYR | A | 213 | 8.751  | 23.051 | 17.589 | 1.00 | 26.74 | C |
| ATOM | 1599 | CE1 | TYR | A | 213 | 6.716  | 21.237 | 18.011 | 1.00 | 28.91 | C |
| ATOM | 1600 | CE2 | TYR | A | 213 | 8.378  | 22.193 | 16.585 | 1.00 | 28.63 | C |
| ATOM | 1601 | CZ  | TYR | A | 213 | 7.366  | 21.295 | 16.795 | 1.00 | 29.44 | C |
| ATOM | 1602 | OH  | TYR | A | 213 | 7.013  | 20.456 | 15.756 | 1.00 | 33.67 | O |
| ATOM | 1603 | N   | LYS | A | 214 | 11.239 | 24.788 | 21.609 | 1.00 | 21.60 | N |
| ATOM | 1604 | CA  | LYS | A | 214 | 11.875 | 25.793 | 22.414 | 1.00 | 21.89 | C |
| ATOM | 1605 | C   | LYS | A | 214 | 12.312 | 26.947 | 21.528 | 1.00 | 21.62 | C |
| ATOM | 1606 | O   | LYS | A | 214 | 12.878 | 26.747 | 20.442 | 1.00 | 22.07 | O |
| ATOM | 1607 | CB  | LYS | A | 214 | 13.103 | 25.239 | 23.140 | 1.00 | 22.10 | C |
| ATOM | 1608 | CG  | LYS | A | 214 | 12.796 | 24.385 | 24.338 | 1.00 | 22.63 | C |
| ATOM | 1609 | CD  | LYS | A | 214 | 14.103 | 23.893 | 24.964 | 1.00 | 24.24 | C |
| ATOM | 1610 | CE  | LYS | A | 214 | 13.923 | 23.478 | 26.402 | 1.00 | 23.54 | C |
| ATOM | 1611 | NZ  | LYS | A | 214 | 15.169 | 22.872 | 26.951 | 1.00 | 22.10 | N |
| ATOM | 1612 | N   | ARG | A | 215 | 12.007 | 28.156 | 21.974 | 1.00 | 20.97 | N |
| ATOM | 1613 | CA  | ARG | A | 215 | 12.447 | 29.347 | 21.277 | 1.00 | 20.73 | C |
| ATOM | 1614 | C   | ARG | A | 215 | 13.778 | 29.724 | 21.900 | 1.00 | 20.03 | C |
| ATOM | 1615 | O   | ARG | A | 215 | 13.885 | 29.828 | 23.113 | 1.00 | 19.70 | O |
| ATOM | 1616 | CB  | ARG | A | 215 | 11.461 | 30.470 | 21.493 | 1.00 | 21.30 | C |
| ATOM | 1617 | CG  | ARG | A | 215 | 11.754 | 31.760 | 20.726 | 1.00 | 22.21 | C |
| ATOM | 1618 | CD  | ARG | A | 215 | 11.177 | 32.925 | 21.473 | 1.00 | 24.71 | C |
| ATOM | 1619 | NE  | ARG | A | 215 | 11.122 | 34.156 | 20.715 | 1.00 | 25.47 | N |
| ATOM | 1620 | CZ  | ARG | A | 215 | 10.479 | 35.235 | 21.130 | 1.00 | 26.28 | C |
| ATOM | 1621 | NH1 | ARG | A | 215 | 9.844  | 35.245 | 22.299 | 1.00 | 26.07 | N |
| ATOM | 1622 | NH2 | ARG | A | 215 | 10.483 | 36.314 | 20.384 | 1.00 | 28.83 | N |
| ATOM | 1623 | N   | CYS | A | 216 | 14.794 | 29.877 | 21.074 | 1.00 | 19.45 | C |
| ATOM | 1624 | CA  | CYS | A | 216 | 16.116 | 30.219 | 21.554 | 1.00 | 19.58 | C |
| ATOM | 1625 | C   | CYS | A | 216 | 16.503 | 31.587 | 20.993 | 1.00 | 19.92 | O |
| ATOM | 1626 | O   | CYS | A | 216 | 16.503 | 31.774 | 19.789 | 1.00 | 20.16 | C |
| ATOM | 1627 | CB  | CYS | A | 216 | 17.110 | 29.186 | 21.073 | 1.00 | 20.01 | S |
| ATOM | 1628 | SG  | CYS | A | 216 | 16.693 | 27.450 | 21.462 | 1.00 | 21.39 | N |
| ATOM | 1629 | N   | ILE | A | 217 | 16.812 | 32.530 | 21.878 | 1.00 | 19.28 | C |
| ATOM | 1630 | CA  | ILE | A | 217 | 17.286 | 33.845 | 21.504 | 1.00 | 19.58 | C |
| ATOM | 1631 | C   | ILE | A | 217 | 18.742 | 33.961 | 21.937 | 1.00 | 19.21 | O |
| ATOM | 1632 | O   | ILE | A | 217 | 19.055 | 33.849 | 23.126 | 1.00 | 19.05 | C |
| ATOM | 1633 | CB  | ILE | A | 217 | 16.424 | 34.943 | 22.168 | 1.00 | 19.88 | C |
| ATOM | 1634 | CG1 | ILE | A | 217 | 14.926 | 34.687 | 21.878 | 1.00 | 20.56 | C |
| ATOM | 1635 | CG2 | ILE | A | 217 | 16.803 | 36.312 | 21.627 | 1.00 | 20.25 | C |
| ATOM | 1636 | CD1 | ILE | A | 217 | 13.984 | 35.692 | 22.488 | 1.00 | 20.99 | C |
| ATOM | 1637 | N   | LEU | A | 218 | 19.620 | 34.176 | 20.965 | 1.00 | 19.01 | N |
| ATOM | 1638 | CA  | LEU | A | 218 | 21.048 | 34.271 | 21.222 | 1.00 | 19.61 | C |
| ATOM | 1639 | C   | LEU | A | 218 | 21.568 | 35.682 | 20.970 | 1.00 | 20.43 | C |
| ATOM | 1640 | O   | LEU | A | 218 | 21.018 | 36.414 | 20.136 | 1.00 | 19.76 | O |
| ATOM | 1641 | CB  | LEU | A | 218 | 21.816 | 33.329 | 20.308 | 1.00 | 19.66 | C |
| ATOM | 1642 | CG  | LEU | A | 218 | 21.906 | 31.881 | 20.778 | 1.00 | 19.74 | C |
| ATOM | 1643 | CD1 | LEU | A | 218 | 20.549 | 31.237 | 20.905 | 1.00 | 20.56 | C |
| ATOM | 1644 | CD2 | LEU | A | 218 | 22.733 | 31.099 | 19.798 | 1.00 | 21.32 | C |
| ATOM | 1645 | N   | PHE | A | 219 | 22.626 | 36.046 | 21.700 | 1.00 | 20.11 | N |
| ATOM | 1646 | CA  | PHE | A | 219 | 23.282 | 37.324 | 21.524 | 1.00 | 20.96 | C |
| ATOM | 1647 | C   | PHE | A | 219 | 24.805 | 37.078 | 21.453 | 1.00 | 21.19 | C |
| ATOM | 1648 | O   | PHE | A | 219 | 25.351 | 36.313 | 22.257 | 1.00 | 21.20 | O |
| ATOM | 1649 | CB  | PHE | A | 219 | 22.942 | 38.304 | 22.678 | 1.00 | 20.97 | C |
| ATOM | 1650 | CG  | PHE | A | 219 | 21.463 | 38.456 | 22.954 | 1.00 | 20.44 | C |
| ATOM | 1651 | CD1 | PHE | A | 219 | 20.821 | 37.637 | 23.846 | 1.00 | 21.46 | C |
| ATOM | 1652 | CD2 | PHE | A | 219 | 20.724 | 39.447 | 22.334 | 1.00 | 22.49 | C |
| ATOM | 1653 | CE1 | PHE | A | 219 | 19.472 | 37.790 | 24.108 | 1.00 | 22.33 | C |
| ATOM | 1654 | CE2 | PHE | A | 219 | 19.387 | 39.605 | 22.605 | 1.00 | 21.32 | C |
| ATOM | 1655 | CZ  | PHE | A | 219 | 18.760 | 38.773 | 23.480 | 1.00 | 21.50 | C |
| ATOM | 1656 | N   | PRO | A | 220 | 25.485 | 37.705 | 20.498 | 1.00 | 21.20 | N |
| ATOM | 1657 | CA  | PRO | A | 220 | 26.936 | 37.541 | 20.368 | 1.00 | 21.72 | C |
| ATOM | 1658 | C   | PRO | A | 220 | 27.683 | 38.108 | 21.569 | 1.00 | 21.31 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1659 | O   | PRO | A | 220 | 27.165 | 38.972 | 22.280 | 1.00 | 20.90 | O |
| ATOM | 1660 | CB  | PRO | A | 220 | 27.302 | 38.341 | 19.120 | 1.00 | 21.41 | C |
| ATOM | 1661 | CG  | PRO | A | 220 | 26.020 | 38.781 | 18.510 | 1.00 | 23.12 | C |
| ATOM | 1662 | CD  | PRO | A | 220 | 24.938 | 38.637 | 19.508 | 1.00 | 22.22 | C |
| ATOM | 1663 | N   | PRO | A | 221 | 28.884 | 37.594 | 21.806 | 1.00 | 21.46 | N |
| ATOM | 1664 | CA  | PRO | A | 221 | 29.721 | 38.053 | 22.918 | 1.00 | 21.33 | C |
| ATOM | 1665 | C   | PRO | A | 221 | 29.961 | 39.556 | 22.940 | 1.00 | 21.04 | C |
| ATOM | 1666 | O   | PRO | A | 221 | 30.220 | 40.096 | 24.009 | 1.00 | 20.68 | O |
| ATOM | 1667 | CB  | PRO | A | 221 | 31.032 | 37.325 | 22.681 | 1.00 | 21.42 | C |
| ATOM | 1668 | CG  | PRO | A | 221 | 30.656 | 36.134 | 21.939 | 1.00 | 22.42 | C |
| ATOM | 1669 | CD  | PRO | A | 221 | 29.522 | 36.510 | 21.041 | 1.00 | 21.53 | C |
| ATOM | 1670 | N   | ASP | A | 222 | 29.877 | 40.225 | 21.792 | 1.00 | 21.47 | N |
| ATOM | 1671 | CA  | ASP | A | 222 | 30.128 | 41.669 | 21.749 | 1.00 | 21.80 | C |
| ATOM | 1672 | C   | ASP | A | 222 | 28.946 | 42.464 | 22.271 | 1.00 | 21.74 | C |
| ATOM | 1673 | O   | ASP | A | 222 | 28.970 | 43.685 | 22.261 | 1.00 | 22.16 | O |
| ATOM | 1674 | CB  | ASP | A | 222 | 30.568 | 42.148 | 20.355 | 1.00 | 21.85 | C |
| ATOM | 1675 | CG  | ASP | A | 222 | 29.433 | 42.151 | 19.325 | 1.00 | 24.83 | C |
| ATOM | 1676 | OD1 | ASP | A | 222 | 28.311 | 41.668 | 19.585 | 1.00 | 25.32 | O |
| ATOM | 1677 | OD2 | ASP | A | 222 | 29.595 | 42.607 | 18.186 | 1.00 | 29.30 | O |
| ATOM | 1678 | N   | GLN | A | 223 | 27.916 | 41.775 | 22.748 | 1.00 | 21.94 | N |
| ATOM | 1679 | CA  | GLN | A | 223 | 26.794 | 42.453 | 23.388 | 1.00 | 22.17 | C |
| ATOM | 1680 | C   | GLN | A | 223 | 26.897 | 42.388 | 24.928 | 1.00 | 21.93 | C |
| ATOM | 1681 | O   | GLN | A | 223 | 25.926 | 42.681 | 25.660 | 1.00 | 21.70 | O |
| ATOM | 1682 | CB  | GLN | A | 223 | 25.456 | 41.911 | 22.832 | 1.00 | 22.84 | C |
| ATOM | 1683 | CG  | GLN | A | 223 | 25.149 | 42.508 | 21.412 | 1.00 | 25.34 | C |
| ATOM | 1684 | CD  | GLN | A | 223 | 23.728 | 42.283 | 20.965 | 1.00 | 27.81 | C |
| ATOM | 1685 | OE1 | GLN | A | 223 | 22.801 | 42.473 | 21.750 | 1.00 | 30.00 | O |
| ATOM | 1686 | NE2 | GLN | A | 223 | 23.543 | 41.850 | 19.709 | 1.00 | 29.69 | N |
| ATOM | 1687 | N   | PHE | A | 224 | 28.079 | 42.027 | 25.417 | 1.00 | 21.04 | N |
| ATOM | 1688 | CA  | PHE | A | 224 | 28.363 | 42.035 | 26.860 | 1.00 | 21.41 | C |
| ATOM | 1689 | C   | PHE | A | 224 | 27.886 | 43.350 | 27.527 | 1.00 | 21.57 | C |
| ATOM | 1690 | O   | PHE | A | 224 | 27.240 | 43.315 | 28.561 | 1.00 | 21.34 | O |
| ATOM | 1691 | CB  | PHE | A | 224 | 29.883 | 41.874 | 27.076 | 1.00 | 20.95 | C |
| ATOM | 1692 | CG  | PHE | A | 224 | 30.304 | 41.773 | 28.529 | 1.00 | 21.82 | C |
| ATOM | 1693 | CD1 | PHE | A | 224 | 30.452 | 42.912 | 29.319 | 1.00 | 19.33 | C |
| ATOM | 1694 | CD2 | PHE | A | 224 | 30.595 | 40.552 | 29.089 | 1.00 | 20.01 | C |
| ATOM | 1695 | CE1 | PHE | A | 224 | 30.870 | 42.807 | 30.630 | 1.00 | 20.89 | C |
| ATOM | 1696 | CE2 | PHE | A | 224 | 31.025 | 40.449 | 30.397 | 1.00 | 20.59 | C |
| ATOM | 1697 | CZ  | PHE | A | 224 | 31.151 | 41.579 | 31.171 | 1.00 | 20.99 | C |
| ATOM | 1698 | N   | GLU | A | 225 | 28.195 | 44.495 | 26.916 | 1.00 | 22.10 | N |
| ATOM | 1699 | CA  | GLU | A | 225 | 27.823 | 45.800 | 27.466 | 1.00 | 23.01 | C |
| ATOM | 1700 | C   | GLU | A | 225 | 26.337 | 46.042 | 27.574 | 1.00 | 22.26 | C |
| ATOM | 1701 | O   | GLU | A | 225 | 25.928 | 46.946 | 28.311 | 1.00 | 21.91 | O |
| ATOM | 1702 | CB  | GLU | A | 225 | 28.401 | 46.935 | 26.624 | 1.00 | 24.27 | C |
| ATOM | 1703 | CG  | GLU | A | 225 | 29.886 | 47.133 | 26.857 | 1.00 | 29.26 | C |
| ATOM | 1704 | CD  | GLU | A | 225 | 30.312 | 48.579 | 27.062 | 1.00 | 35.91 | C |
| ATOM | 1705 | OE1 | GLU | A | 225 | 29.745 | 49.317 | 27.942 | 1.00 | 39.92 | O |
| ATOM | 1706 | OE2 | GLU | A | 225 | 31.281 | 48.958 | 26.368 | 1.00 | 40.78 | O |
| ATOM | 1707 | N   | CYS | A | 226 | 25.539 | 45.258 | 26.836 | 1.00 | 21.15 | N |
| ATOM | 1708 | CA  | CYS | A | 226 | 24.081 | 45.396 | 26.851 | 1.00 | 21.01 | C |
| ATOM | 1709 | C   | CYS | A | 226 | 23.359 | 44.417 | 27.768 | 1.00 | 20.67 | C |
| ATOM | 1710 | O   | CYS | A | 226 | 22.159 | 44.601 | 28.043 | 1.00 | 18.85 | O |
| ATOM | 1711 | CB  | CYS | A | 226 | 23.520 | 45.190 | 25.447 | 1.00 | 20.88 | C |
| ATOM | 1712 | SG  | CYS | A | 226 | 24.194 | 46.296 | 24.190 | 1.00 | 22.39 | S |
| ATOM | 1713 | N   | LEU | A | 227 | 24.085 | 43.399 | 28.256 | 1.00 | 20.56 | N |
| ATOM | 1714 | CA  | LEU | A | 227 | 23.461 | 42.304 | 28.985 | 1.00 | 20.48 | C |
| ATOM | 1715 | C   | LEU | A | 227 | 23.795 | 42.185 | 30.466 | 1.00 | 20.42 | C |
| ATOM | 1716 | O   | LEU | A | 227 | 23.180 | 41.398 | 31.187 | 1.00 | 20.78 | O |
| ATOM | 1717 | CB  | LEU | A | 227 | 23.737 | 41.003 | 28.232 | 1.00 | 21.20 | C |
| ATOM | 1718 | CG  | LEU | A | 227 | 22.865 | 40.993 | 26.963 | 1.00 | 22.96 | C |
| ATOM | 1719 | CD1 | LEU | A | 227 | 23.373 | 40.023 | 25.929 | 1.00 | 24.99 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1720 | CD2 | LEU | A | 227 | 21.420 | 40.655 | 27.323 | 1.00 | 24.79 | C |
| ATOM | 1721 | N   | TYR | A | 228 | 24.793 | 42.939 | 30.901 | 1.00 | 20.08 | N |
| ATOM | 1722 | CA  | TYR | A | 228 | 25.060 | 43.127 | 32.303 | 1.00 | 19.66 | C |
| ATOM | 1723 | C   | TYR | A | 228 | 25.061 | 41.858 | 33.165 | 1.00 | 19.95 | C |
| ATOM | 1724 | O   | TYR | A | 228 | 24.229 | 41.697 | 34.058 | 1.00 | 19.69 | O |
| ATOM | 1725 | CB  | TYR | A | 228 | 24.050 | 44.137 | 32.857 | 1.00 | 19.77 | C |
| ATOM | 1726 | CG  | TYR | A | 228 | 24.028 | 45.481 | 32.119 | 1.00 | 19.37 | C |
| ATOM | 1727 | CD1 | TYR | A | 228 | 24.836 | 46.513 | 32.515 | 1.00 | 18.65 | C |
| ATOM | 1728 | CD2 | TYR | A | 228 | 23.180 | 45.697 | 31.036 | 1.00 | 19.82 | C |
| ATOM | 1729 | CE1 | TYR | A | 228 | 24.819 | 47.759 | 31.862 | 1.00 | 20.56 | C |
| ATOM | 1730 | CE2 | TYR | A | 228 | 23.143 | 46.920 | 30.380 | 1.00 | 20.78 | C |
| ATOM | 1731 | CZ  | TYR | A | 228 | 23.962 | 47.956 | 30.801 | 1.00 | 20.88 | C |
| ATOM | 1732 | OH  | TYR | A | 228 | 23.944 | 49.174 | 30.152 | 1.00 | 19.73 | O |
| ATOM | 1733 | N   | PRO | A | 229 | 26.028 | 40.981 | 32.941 | 1.00 | 19.99 | N |
| ATOM | 1734 | CA  | PRO | A | 229 | 26.140 | 39.781 | 33.768 | 1.00 | 20.44 | C |
| ATOM | 1735 | C   | PRO | A | 229 | 26.481 | 40.141 | 35.196 | 1.00 | 19.99 | C |
| ATOM | 1736 | O   | PRO | A | 229 | 27.130 | 41.166 | 35.451 | 1.00 | 20.03 | O |
| ATOM | 1737 | CB  | PRO | A | 229 | 27.334 | 39.043 | 33.157 | 1.00 | 20.11 | C |
| ATOM | 1738 | CG  | PRO | A | 229 | 28.125 | 40.130 | 32.541 | 1.00 | 21.04 | C |
| ATOM | 1739 | CD  | PRO | A | 229 | 27.099 | 41.050 | 31.935 | 1.00 | 19.79 | C |
| ATOM | 1740 | N   | TYR | A | 230 | 26.044 | 39.294 | 36.115 | 1.00 | 19.50 | N |
| ATOM | 1741 | CA  | TYR | A | 230 | 26.348 | 39.458 | 37.511 | 1.00 | 19.17 | C |
| ATOM | 1742 | C   | TYR | A | 230 | 27.860 | 39.464 | 37.704 | 1.00 | 19.14 | C |
| ATOM | 1743 | O   | TYR | A | 230 | 28.598 | 39.060 | 36.832 | 1.00 | 18.83 | O |
| ATOM | 1744 | CB  | TYR | A | 230 | 25.746 | 38.313 | 38.320 | 1.00 | 18.51 | C |
| ATOM | 1745 | CG  | TYR | A | 230 | 24.253 | 38.411 | 38.531 | 1.00 | 18.95 | C |
| ATOM | 1746 | CD1 | TYR | A | 230 | 23.368 | 37.949 | 37.560 | 1.00 | 18.39 | C |
| ATOM | 1747 | CD2 | TYR | A | 230 | 23.719 | 38.969 | 39.707 | 1.00 | 18.65 | C |
| ATOM | 1748 | CE1 | TYR | A | 230 | 22.001 | 38.006 | 37.751 | 1.00 | 17.34 | C |
| ATOM | 1749 | CE2 | TYR | A | 230 | 22.337 | 39.043 | 39.903 | 1.00 | 17.05 | C |
| ATOM | 1750 | CZ  | TYR | A | 230 | 21.492 | 38.550 | 38.909 | 1.00 | 17.79 | C |
| ATOM | 1751 | OH  | TYR | A | 230 | 20.127 | 38.601 | 39.051 | 1.00 | 19.77 | O |
| ATOM | 1752 | N   | PRO | A | 231 | 28.316 | 39.963 | 38.843 | 1.00 | 19.95 | N |
| ATOM | 1753 | CA  | PRO | A | 231 | 29.722 | 39.829 | 39.213 | 1.00 | 20.42 | C |
| ATOM | 1754 | C   | PRO | A | 231 | 30.157 | 38.339 | 39.187 | 1.00 | 20.93 | C |
| ATOM | 1755 | O   | PRO | A | 231 | 29.345 | 37.463 | 39.506 | 1.00 | 20.71 | O |
| ATOM | 1756 | CB  | PRO | A | 231 | 29.755 | 40.369 | 40.642 | 1.00 | 20.70 | C |
| ATOM | 1757 | CG  | PRO | A | 231 | 28.588 | 41.341 | 40.716 | 1.00 | 20.76 | C |
| ATOM | 1758 | CD  | PRO | A | 231 | 27.528 | 40.701 | 39.845 | 1.00 | 19.53 | C |
| ATOM | 1759 | N   | VAL | A | 232 | 31.413 | 38.067 | 38.831 | 1.00 | 20.93 | N |
| ATOM | 1760 | CA  | VAL | A | 232 | 31.906 | 36.685 | 38.742 | 1.00 | 21.31 | C |
| ATOM | 1761 | C   | VAL | A | 232 | 31.722 | 35.843 | 40.014 | 1.00 | 20.95 | C |
| ATOM | 1762 | O   | VAL | A | 232 | 31.431 | 34.650 | 39.934 | 1.00 | 20.50 | O |
| ATOM | 1763 | CB  | VAL | A | 232 | 33.398 | 36.655 | 38.304 | 1.00 | 21.35 | C |
| ATOM | 1764 | CG1 | VAL | A | 232 | 34.029 | 35.280 | 38.552 | 1.00 | 22.23 | C |
| ATOM | 1765 | CG2 | VAL | A | 232 | 33.533 | 37.031 | 36.850 | 1.00 | 21.71 | C |
| ATOM | 1766 | N   | HIS | A | 233 | 31.872 | 36.455 | 41.181 | 1.00 | 21.10 | N |
| ATOM | 1767 | CA  | HIS | A | 233 | 31.742 | 35.721 | 42.438 | 1.00 | 21.01 | C |
| ATOM | 1768 | C   | HIS | A | 233 | 30.302 | 35.571 | 42.944 | 1.00 | 20.95 | C |
| ATOM | 1769 | O   | HIS | A | 233 | 30.045 | 34.864 | 43.914 | 1.00 | 19.92 | O |
| ATOM | 1770 | CB  | HIS | A | 233 | 32.606 | 36.363 | 43.501 | 1.00 | 21.12 | C |
| ATOM | 1771 | CG  | HIS | A | 233 | 34.063 | 36.342 | 43.174 | 1.00 | 21.52 | C |
| ATOM | 1772 | ND1 | HIS | A | 233 | 34.720 | 37.424 | 42.625 | 1.00 | 22.78 | N |
| ATOM | 1773 | CD2 | HIS | A | 233 | 34.993 | 35.368 | 43.318 | 1.00 | 22.27 | C |
| ATOM | 1774 | CE1 | HIS | A | 233 | 35.994 | 37.114 | 42.446 | 1.00 | 24.00 | C |
| ATOM | 1775 | NE2 | HIS | A | 233 | 36.186 | 35.870 | 42.857 | 1.00 | 23.34 | N |
| ATOM | 1776 | N   | HIS | A | 234 | 29.364 | 36.236 | 42.288 | 1.00 | 20.94 | N |
| ATOM | 1777 | CA  | HIS | A | 234 | 27.959 | 36.081 | 42.630 | 1.00 | 21.27 | C |
| ATOM | 1778 | C   | HIS | A | 234 | 27.493 | 34.722 | 42.103 | 1.00 | 21.28 | C |
| ATOM | 1779 | O   | HIS | A | 234 | 28.022 | 34.233 | 41.107 | 1.00 | 21.02 | O |
| ATOM | 1780 | CB  | HIS | A | 234 | 27.169 | 37.203 | 41.989 | 1.00 | 21.52 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1781 | CG  | HIS | A | 234 | 25.730 | 37.253 | 42.374 | 1.00 | 21.54 | C |
| ATOM | 1782 | ND1 | HIS | A | 234 | 24.769 | 36.498 | 41.740 | 1.00 | 21.95 | N |
| ATOM | 1783 | CD2 | HIS | A | 234 | 25.073 | 38.028 | 43.269 | 1.00 | 22.67 | C |
| ATOM | 1784 | CE1 | HIS | A | 234 | 23.585 | 36.779 | 42.254 | 1.00 | 22.38 | C |
| ATOM | 1785 | NE2 | HIS | A | 234 | 23.743 | 37.700 | 43.187 | 1.00 | 21.91 | N |
| ATOM | 1786 | N   | PRO | A | 235 | 26.551 | 34.087 | 42.792 | 1.00 | 21.11 | N |
| ATOM | 1787 | CA  | PRO | A | 235 | 25.999 | 32.809 | 42.338 | 1.00 | 21.46 | C |
| ATOM | 1788 | C   | PRO | A | 235 | 25.461 | 32.835 | 40.916 | 1.00 | 21.10 | C |
| ATOM | 1789 | O   | PRO | A | 235 | 25.517 | 31.802 | 40.244 | 1.00 | 20.37 | O |
| ATOM | 1790 | CB  | PRO | A | 235 | 24.860 | 32.551 | 43.325 | 1.00 | 21.90 | C |
| ATOM | 1791 | CG  | PRO | A | 235 | 25.316 | 33.240 | 44.574 | 1.00 | 22.00 | C |
| ATOM | 1792 | CD  | PRO | A | 235 | 26.007 | 34.485 | 44.100 | 1.00 | 21.41 | C |
| ATOM | 1793 | N   | CYS | A | 236 | 24.997 | 33.989 | 40.452 | 1.00 | 20.41 | N |
| ATOM | 1794 | CA  | CYS | A | 236 | 24.456 | 34.077 | 39.110 | 1.00 | 20.17 | C |
| ATOM | 1795 | C   | CYS | A | 236 | 25.503 | 34.554 | 38.107 | 1.00 | 20.00 | C |
| ATOM | 1796 | O   | CYS | A | 236 | 25.180 | 35.111 | 37.061 | 1.00 | 20.30 | O |
| ATOM | 1797 | CB  | CYS | A | 236 | 23.195 | 34.924 | 39.090 | 1.00 | 19.66 | C |
| ATOM | 1798 | SG  | CYS | A | 236 | 21.914 | 34.209 | 40.133 | 1.00 | 20.71 | S |
| ATOM | 1799 | N   | ASP | A | 237 | 26.768 | 34.311 | 38.433 | 1.00 | 19.87 | N |
| ATOM | 1800 | CA  | ASP | A | 237 | 27.857 | 34.498 | 37.485 | 1.00 | 19.60 | C |
| ATOM | 1801 | C   | ASP | A | 237 | 27.459 | 33.915 | 36.105 | 1.00 | 19.48 | C |
| ATOM | 1802 | O   | ASP | A | 237 | 26.883 | 32.834 | 36.020 | 1.00 | 18.94 | O |
| ATOM | 1803 | CB  | ASP | A | 237 | 29.075 | 33.789 | 38.031 | 1.00 | 19.20 | C |
| ATOM | 1804 | CG  | ASP | A | 237 | 30.268 | 33.842 | 37.107 | 1.00 | 20.58 | C |
| ATOM | 1805 | OD1 | ASP | A | 237 | 30.477 | 34.871 | 36.373 | 1.00 | 18.56 | O |
| ATOM | 1806 | OD2 | ASP | A | 237 | 31.070 | 32.868 | 37.077 | 1.00 | 19.51 | O |
| ATOM | 1807 | N   | ARG | A | 238 | 27.749 | 34.675 | 35.056 | 1.00 | 19.85 | N |
| ATOM | 1808 | CA  | ARG | A | 238 | 27.459 | 34.332 | 33.664 | 1.00 | 20.90 | C |
| ATOM | 1809 | C   | ARG | A | 238 | 26.002 | 34.572 | 33.247 | 1.00 | 20.67 | C |
| ATOM | 1810 | O   | ARG | A | 238 | 25.709 | 34.491 | 32.059 | 1.00 | 21.20 | O |
| ATOM | 1811 | CB  | ARG | A | 238 | 27.854 | 32.876 | 33.319 | 1.00 | 21.44 | C |
| ATOM | 1812 | CG  | ARG | A | 238 | 29.330 | 32.585 | 33.482 | 1.00 | 21.04 | C |
| ATOM | 1813 | CD  | ARG | A | 238 | 29.710 | 31.150 | 33.145 | 1.00 | 22.38 | C |
| ATOM | 1814 | NE  | ARG | A | 238 | 29.080 | 30.243 | 34.085 | 1.00 | 23.86 | N |
| ATOM | 1815 | CZ  | ARG | A | 238 | 27.937 | 29.584 | 33.874 | 1.00 | 25.81 | C |
| ATOM | 1816 | NH1 | ARG | A | 238 | 27.262 | 29.686 | 32.712 | 1.00 | 24.18 | N |
| ATOM | 1817 | NH2 | ARG | A | 238 | 27.471 | 28.810 | 34.849 | 1.00 | 27.18 | N |
| ATOM | 1818 | N   | GLN | A | 239 | 25.105 | 34.845 | 34.190 | 1.00 | 19.94 | N |
| ATOM | 1819 | CA  | GLN | A | 239 | 23.722 | 35.141 | 33.833 | 1.00 | 20.58 | C |
| ATOM | 1820 | C   | GLN | A | 239 | 23.535 | 36.661 | 33.740 | 1.00 | 20.50 | C |
| ATOM | 1821 | O   | GLN | A | 239 | 24.219 | 37.402 | 34.446 | 1.00 | 20.63 | O |
| ATOM | 1822 | CB  | GLN | A | 239 | 22.735 | 34.591 | 34.863 | 1.00 | 20.32 | C |
| ATOM | 1823 | CG  | GLN | A | 239 | 23.159 | 33.314 | 35.594 | 1.00 | 20.84 | C |
| ATOM | 1824 | CD  | GLN | A | 239 | 23.367 | 32.137 | 34.673 | 1.00 | 21.23 | C |
| ATOM | 1825 | OE1 | GLN | A | 239 | 22.434 | 31.675 | 34.014 | 1.00 | 21.22 | O |
| ATOM | 1826 | NE2 | GLN | A | 239 | 24.591 | 31.655 | 34.616 | 1.00 | 20.93 | N |
| ATOM | 1827 | N   | SER | A | 240 | 22.600 | 37.112 | 32.900 | 1.00 | 20.07 | N |
| ATOM | 1828 | CA  | SER | A | 240 | 22.282 | 38.533 | 32.768 | 1.00 | 20.18 | C |
| ATOM | 1829 | C   | SER | A | 240 | 21.498 | 39.027 | 33.969 | 1.00 | 20.71 | C |
| ATOM | 1830 | O   | SER | A | 240 | 20.619 | 38.316 | 34.467 | 1.00 | 20.85 | O |
| ATOM | 1831 | CB  | SER | A | 240 | 21.405 | 38.776 | 31.539 | 1.00 | 20.29 | C |
| ATOM | 1832 | OG  | SER | A | 240 | 21.007 | 40.137 | 31.454 | 1.00 | 21.43 | O |
| ATOM | 1833 | N   | GLN | A | 241 | 21.793 | 40.246 | 34.426 | 1.00 | 20.46 | N |
| ATOM | 1834 | CA  | GLN | A | 241 | 21.013 | 40.839 | 35.496 | 1.00 | 20.42 | C |
| ATOM | 1835 | C   | GLN | A | 241 | 19.711 | 41.433 | 34.965 | 1.00 | 20.26 | C |
| ATOM | 1836 | O   | GLN | A | 241 | 18.839 | 41.767 | 35.726 | 1.00 | 19.62 | O |
| ATOM | 1837 | CB  | GLN | A | 241 | 21.770 | 41.949 | 36.201 | 1.00 | 20.32 | C |
| ATOM | 1838 | CG  | GLN | A | 241 | 23.019 | 41.544 | 36.912 | 1.00 | 20.58 | C |
| ATOM | 1839 | CD  | GLN | A | 241 | 23.771 | 42.767 | 37.423 | 1.00 | 21.94 | C |
| ATOM | 1840 | OE1 | GLN | A | 241 | 23.524 | 43.210 | 38.514 | 1.00 | 23.52 | O |
| ATOM | 1841 | NE2 | GLN | A | 241 | 24.670 | 43.304 | 36.624 | 1.00 | 20.84 | N |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1842 | N   | VAL | A | 242 | 19.557 | 41.563 | 33.659 | 1.00 | 20.57 | N |
| ATOM | 1843 | CA  | VAL | A | 242 | 18.361 | 42.229 | 33.182 | 1.00 | 20.73 | C |
| ATOM | 1844 | C   | VAL | A | 242 | 17.173 | 41.309 | 33.246 | 1.00 | 20.69 | C |
| ATOM | 1845 | O   | VAL | A | 242 | 17.244 | 40.190 | 32.757 | 1.00 | 21.13 | O |
| ATOM | 1846 | CB  | VAL | A | 242 | 18.498 | 42.667 | 31.712 | 1.00 | 21.03 | C |
| ATOM | 1847 | CG1 | VAL | A | 242 | 17.204 | 43.377 | 31.250 | 1.00 | 20.85 | C |
| ATOM | 1848 | CG2 | VAL | A | 242 | 19.723 | 43.527 | 31.498 | 1.00 | 20.71 | C |
| ATOM | 1849 | N   | ASP | A | 243 | 16.071 | 41.786 | 33.813 | 1.00 | 20.62 | N |
| ATOM | 1850 | CA  | ASP | A | 243 | 14.807 | 41.042 | 33.788 | 1.00 | 20.64 | C |
| ATOM | 1851 | C   | ASP | A | 243 | 14.148 | 41.348 | 32.448 | 1.00 | 20.94 | C |
| ATOM | 1852 | O   | ASP | A | 243 | 13.591 | 42.438 | 32.230 | 1.00 | 19.75 | O |
| ATOM | 1853 | CB  | ASP | A | 243 | 13.916 | 41.471 | 34.963 | 1.00 | 20.88 | C |
| ATOM | 1854 | CG  | ASP | A | 243 | 12.526 | 40.894 | 34.898 | 1.00 | 21.39 | C |
| ATOM | 1855 | OD1 | ASP | A | 243 | 12.209 | 40.153 | 33.941 | 1.00 | 23.25 | O |
| ATOM | 1856 | OD2 | ASP | A | 243 | 11.672 | 41.130 | 35.784 | 1.00 | 23.49 | O |
| ATOM | 1857 | N   | PHE | A | 244 | 14.238 | 40.385 | 31.541 | 1.00 | 21.19 | N |
| ATOM | 1858 | CA  | PHE | A | 244 | 13.717 | 40.549 | 30.197 | 1.00 | 21.56 | C |
| ATOM | 1859 | C   | PHE | A | 244 | 12.225 | 40.916 | 30.204 | 1.00 | 22.49 | C |
| ATOM | 1860 | O   | PHE | A | 244 | 11.734 | 41.521 | 29.260 | 1.00 | 21.85 | O |
| ATOM | 1861 | CB  | PHE | A | 244 | 13.940 | 39.275 | 29.378 | 1.00 | 21.85 | C |
| ATOM | 1862 | CG  | PHE | A | 244 | 15.316 | 39.152 | 28.743 | 1.00 | 20.87 | C |
| ATOM | 1863 | CD1 | PHE | A | 244 | 16.457 | 39.540 | 29.399 | 1.00 | 20.74 | C |
| ATOM | 1864 | CD2 | PHE | A | 244 | 15.446 | 38.617 | 27.483 | 1.00 | 21.00 | C |
| ATOM | 1865 | CE1 | PHE | A | 244 | 17.691 | 39.407 | 28.810 | 1.00 | 19.77 | C |
| ATOM | 1866 | CE2 | PHE | A | 244 | 16.687 | 38.470 | 26.890 | 1.00 | 20.94 | C |
| ATOM | 1867 | CZ  | PHE | A | 244 | 17.805 | 38.881 | 27.551 | 1.00 | 20.34 | C |
| ATOM | 1868 | N   | ASP | A | 245 | 11.500 | 40.554 | 31.259 | 1.00 | 23.56 | N |
| ATOM | 1869 | CA  | ASP | A | 245 | 10.072 | 40.831 | 31.311 | 1.00 | 24.26 | C |
| ATOM | 1870 | C   | ASP | A | 245 | 9.794  | 42.256 | 31.814 | 1.00 | 24.66 | C |
| ATOM | 1871 | O   | ASP | A | 245 | 8.711  | 42.762 | 31.607 | 1.00 | 24.21 | O |
| ATOM | 1872 | CB  | ASP | A | 245 | 9.353  | 39.841 | 32.222 | 1.00 | 24.74 | C |
| ATOM | 1873 | CG  | ASP | A | 245 | 9.408  | 38.427 | 31.721 | 1.00 | 26.56 | C |
| ATOM | 1874 | OD1 | ASP | A | 245 | 9.368  | 38.210 | 30.493 | 1.00 | 28.81 | O |
| ATOM | 1875 | OD2 | ASP | A | 245 | 9.489  | 37.455 | 32.498 | 1.00 | 28.39 | O |
| ATOM | 1876 | N   | ASN | A | 246 | 10.758 | 42.876 | 32.492 | 1.00 | 24.80 | N |
| ATOM | 1877 | CA  | ASN | A | 246 | 10.605 | 44.244 | 32.989 | 1.00 | 25.56 | C |
| ATOM | 1878 | C   | ASN | A | 246 | 11.960 | 44.902 | 33.106 | 1.00 | 25.31 | C |
| ATOM | 1879 | O   | ASN | A | 246 | 12.500 | 45.064 | 34.205 | 1.00 | 25.43 | O |
| ATOM | 1880 | CB  | ASN | A | 246 | 9.912  | 44.285 | 34.345 | 1.00 | 26.09 | C |
| ATOM | 1881 | CG  | ASN | A | 246 | 9.555  | 45.716 | 34.765 | 1.00 | 29.59 | C |
| ATOM | 1882 | OD1 | ASN | A | 246 | 9.366  | 46.598 | 33.912 | 1.00 | 32.67 | O |
| ATOM | 1883 | ND2 | ASN | A | 246 | 9.468  | 45.954 | 36.075 | 1.00 | 33.42 | N |
| ATOM | 1884 | N   | PRO | A | 247 | 12.525 | 45.257 | 31.961 | 1.00 | 25.08 | N |
| ATOM | 1885 | CA  | PRO | A | 247 | 13.885 | 45.782 | 31.911 | 1.00 | 24.89 | C |
| ATOM | 1886 | C   | PRO | A | 247 | 13.992 | 47.144 | 32.579 | 1.00 | 24.95 | C |
| ATOM | 1887 | O   | PRO | A | 247 | 13.217 | 48.049 | 32.297 | 1.00 | 24.55 | O |
| ATOM | 1888 | CB  | PRO | A | 247 | 14.182 | 45.899 | 30.413 | 1.00 | 25.05 | C |
| ATOM | 1889 | CG  | PRO | A | 247 | 13.016 | 45.325 | 29.702 | 1.00 | 25.39 | C |
| ATOM | 1890 | CD  | PRO | A | 247 | 11.890 | 45.184 | 30.640 | 1.00 | 25.02 | C |
| ATOM | 1891 | N   | ASP | A | 248 | 14.976 | 47.267 | 33.460 | 1.00 | 24.53 | N |
| ATOM | 1892 | CA  | ASP | A | 248 | 15.216 | 48.489 | 34.167 | 1.00 | 24.65 | C |
| ATOM | 1893 | C   | ASP | A | 248 | 16.271 | 49.284 | 33.389 | 1.00 | 24.54 | C |
| ATOM | 1894 | O   | ASP | A | 248 | 17.472 | 49.077 | 33.552 | 1.00 | 23.15 | O |
| ATOM | 1895 | CB  | ASP | A | 248 | 15.706 | 48.144 | 35.564 | 1.00 | 24.64 | C |
| ATOM | 1896 | CG  | ASP | A | 248 | 15.787 | 49.343 | 36.454 | 1.00 | 26.02 | C |
| ATOM | 1897 | OD1 | ASP | A | 248 | 16.035 | 50.466 | 35.944 | 1.00 | 26.95 | O |
| ATOM | 1898 | OD2 | ASP | A | 248 | 15.609 | 49.249 | 37.684 | 1.00 | 27.69 | O |
| ATOM | 1899 | N   | TYR | A | 249 | 15.812 | 50.181 | 32.525 | 1.00 | 24.81 | N |
| ATOM | 1900 | CA  | TYR | A | 249 | 16.720 | 50.936 | 31.673 | 1.00 | 25.45 | C |
| ATOM | 1901 | C   | TYR | A | 249 | 17.573 | 51.954 | 32.426 | 1.00 | 25.90 | C |
| ATOM | 1902 | O   | TYR | A | 249 | 18.585 | 52.421 | 31.897 | 1.00 | 25.80 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1903 | CB  | TYR | A | 249 | 15.948 | 51.615 | 30.544 | 1.00 | 25.57 | C |
| ATOM | 1904 | CG  | TYR | A | 249 | 15.244 | 50.651 | 29.630 | 1.00 | 24.58 | C |
| ATOM | 1905 | CD1 | TYR | A | 249 | 15.930 | 49.624 | 29.003 | 1.00 | 25.44 | C |
| ATOM | 1906 | CD2 | TYR | A | 249 | 13.890 | 50.764 | 29.404 | 1.00 | 24.48 | C |
| ATOM | 1907 | CE1 | TYR | A | 249 | 15.276 | 48.731 | 28.173 | 1.00 | 25.01 | C |
| ATOM | 1908 | CE2 | TYR | A | 249 | 13.234 | 49.892 | 28.583 | 1.00 | 24.43 | C |
| ATOM | 1909 | CZ  | TYR | A | 249 | 13.927 | 48.883 | 27.969 | 1.00 | 24.47 | C |
| ATOM | 1910 | OH  | TYR | A | 249 | 13.252 | 48.043 | 27.142 | 1.00 | 25.97 | O |
| ATOM | 1911 | N   | GLU | A | 250 | 17.195 | 52.278 | 33.660 | 1.00 | 26.10 | N |
| ATOM | 1912 | CA  | GLU | A | 250 | 17.999 | 53.190 | 34.458 | 1.00 | 26.93 | C |
| ATOM | 1913 | C   | GLU | A | 250 | 19.259 | 52.492 | 34.929 | 1.00 | 25.85 | C |
| ATOM | 1914 | O   | GLU | A | 250 | 20.329 | 53.086 | 34.964 | 1.00 | 25.90 | O |
| ATOM | 1915 | CB  | GLU | A | 250 | 17.219 | 53.740 | 35.661 | 1.00 | 27.56 | C |
| ATOM | 1916 | CG  | GLU | A | 250 | 16.021 | 54.576 | 35.246 | 1.00 | 32.34 | C |
| ATOM | 1917 | CD  | GLU | A | 250 | 15.420 | 55.366 | 36.385 | 1.00 | 36.85 | C |
| ATOM | 1918 | OE1 | GLU | A | 250 | 15.945 | 55.309 | 37.516 | 1.00 | 42.35 | O |
| ATOM | 1919 | OE2 | GLU | A | 250 | 14.422 | 56.057 | 36.142 | 1.00 | 40.82 | O |
| ATOM | 1920 | N   | ARG | A | 251 | 19.136 | 51.233 | 35.315 | 1.00 | 24.58 | N |
| ATOM | 1921 | CA  | ARG | A | 251 | 20.297 | 50.502 | 35.756 | 1.00 | 23.76 | C |
| ATOM | 1922 | C   | ARG | A | 251 | 21.030 | 49.909 | 34.568 | 1.00 | 22.91 | C |
| ATOM | 1923 | O   | ARG | A | 251 | 22.242 | 49.773 | 34.602 | 1.00 | 22.42 | O |
| ATOM | 1924 | CB  | ARG | A | 251 | 19.896 | 49.374 | 36.696 | 1.00 | 24.55 | C |
| ATOM | 1925 | CG  | ARG | A | 251 | 19.421 | 49.802 | 38.077 | 1.00 | 25.88 | C |
| ATOM | 1926 | CD  | ARG | A | 251 | 18.894 | 48.629 | 38.921 | 1.00 | 29.50 | C |
| ATOM | 1927 | NE  | ARG | A | 251 | 19.993 | 47.764 | 39.349 | 1.00 | 31.63 | N |
| ATOM | 1928 | CZ  | ARG | A | 251 | 19.894 | 46.467 | 39.623 | 1.00 | 33.13 | C |
| ATOM | 1929 | NH1 | ARG | A | 251 | 18.736 | 45.826 | 39.521 | 1.00 | 33.12 | N |
| ATOM | 1930 | NH2 | ARG | A | 251 | 20.978 | 45.805 | 39.998 | 1.00 | 33.93 | N |
| ATOM | 1931 | N   | PHE | A | 252 | 20.300 | 49.560 | 33.515 | 1.00 | 21.47 | N |
| ATOM | 1932 | CA  | PHE | A | 252 | 20.898 | 48.863 | 32.379 | 1.00 | 21.32 | C |
| ATOM | 1933 | C   | PHE | A | 252 | 20.576 | 49.552 | 31.056 | 1.00 | 20.68 | C |
| ATOM | 1934 | O   | PHE | A | 252 | 19.934 | 48.984 | 30.187 | 1.00 | 20.79 | O |
| ATOM | 1935 | CB  | PHE | A | 252 | 20.355 | 47.434 | 32.344 | 1.00 | 21.09 | C |
| ATOM | 1936 | CG  | PHE | A | 252 | 20.373 | 46.738 | 33.690 | 1.00 | 20.96 | C |
| ATOM | 1937 | CD1 | PHE | A | 252 | 21.555 | 46.560 | 34.376 | 1.00 | 19.28 | C |
| ATOM | 1938 | CD2 | PHE | A | 252 | 19.207 | 46.238 | 34.247 | 1.00 | 21.43 | C |
| ATOM | 1939 | CE1 | PHE | A | 252 | 21.571 | 45.891 | 35.609 | 1.00 | 20.54 | C |
| ATOM | 1940 | CE2 | PHE | A | 252 | 19.217 | 45.588 | 35.488 | 1.00 | 22.13 | C |
| ATOM | 1941 | CZ  | PHE | A | 252 | 20.403 | 45.414 | 36.156 | 1.00 | 20.96 | C |
| ATOM | 1942 | N   | PRO | A | 253 | 21.057 | 50.767 | 30.884 | 1.00 | 20.56 | N |
| ATOM | 1943 | CA  | PRO | A | 253 | 20.658 | 51.566 | 29.714 | 1.00 | 20.38 | C |
| ATOM | 1944 | C   | PRO | A | 253 | 20.984 | 50.916 | 28.361 | 1.00 | 20.20 | C |
| ATOM | 1945 | O   | PRO | A | 253 | 20.191 | 51.053 | 27.428 | 1.00 | 19.48 | O |
| ATOM | 1946 | CB  | PRO | A | 253 | 21.383 | 52.903 | 29.928 | 1.00 | 19.77 | C |
| ATOM | 1947 | CG  | PRO | A | 253 | 22.562 | 52.555 | 30.895 | 1.00 | 20.60 | C |
| ATOM | 1948 | CD  | PRO | A | 253 | 21.986 | 51.484 | 31.782 | 1.00 | 20.69 | C |
| ATOM | 1949 | N   | ASN | A | 254 | 22.091 | 50.187 | 28.240 | 1.00 | 20.32 | N |
| ATOM | 1950 | CA  | ASN | A | 254 | 22.409 | 49.613 | 26.938 | 1.00 | 20.12 | C |
| ATOM | 1951 | C   | ASN | A | 254 | 21.572 | 48.393 | 26.554 | 1.00 | 19.96 | C |
| ATOM | 1952 | O   | ASN | A | 254 | 21.675 | 47.892 | 25.441 | 1.00 | 19.16 | O |
| ATOM | 1953 | CB  | ASN | A | 254 | 23.893 | 49.336 | 26.784 | 1.00 | 20.06 | C |
| ATOM | 1954 | CG  | ASN | A | 254 | 24.706 | 50.601 | 26.697 | 1.00 | 21.51 | C |
| ATOM | 1955 | OD1 | ASN | A | 254 | 25.502 | 50.896 | 27.598 | 1.00 | 23.96 | O |
| ATOM | 1956 | ND2 | ASN | A | 254 | 24.514 | 51.373 | 25.614 | 1.00 | 20.38 | N |
| ATOM | 1957 | N   | PHE | A | 255 | 20.724 | 47.922 | 27.455 | 1.00 | 19.81 | N |
| ATOM | 1958 | CA  | PHE | A | 255 | 19.807 | 46.858 | 27.063 | 1.00 | 19.54 | C |
| ATOM | 1959 | C   | PHE | A | 255 | 18.855 | 47.384 | 25.977 | 1.00 | 19.69 | C |
| ATOM | 1960 | O   | PHE | A | 255 | 18.194 | 46.606 | 25.274 | 1.00 | 19.77 | O |
| ATOM | 1961 | CB  | PHE | A | 255 | 19.023 | 46.330 | 28.252 | 1.00 | 19.22 | C |
| ATOM | 1962 | CG  | PHE | A | 255 | 18.269 | 45.105 | 27.940 | 1.00 | 20.47 | C |
| ATOM | 1963 | CD1 | PHE | A | 255 | 18.928 | 43.922 | 27.736 | 1.00 | 20.23 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1964 | CD2 | PHE | A | 255 | 16.909 | 45.148 | 27.758 | 1.00 | 20.13 | C |
| ATOM | 1965 | CE1 | PHE | A | 255 | 18.243 | 42.786 | 27.416 | 1.00 | 21.65 | C |
| ATOM | 1966 | CE2 | PHE | A | 255 | 16.227 | 44.023 | 27.432 | 1.00 | 20.73 | C |
| ATOM | 1967 | CZ  | PHE | A | 255 | 16.886 | 42.842 | 27.257 | 1.00 | 22.63 | C |
| ATOM | 1968 | N   | GLN | A | 256 | 18.790 | 48.707 | 25.841 | 1.00 | 19.89 | N |
| ATOM | 1969 | CA  | GLN | A | 256 | 17.969 | 49.345 | 24.794 | 1.00 | 20.24 | C |
| ATOM | 1970 | C   | GLN | A | 256 | 18.595 | 49.160 | 23.403 | 1.00 | 19.74 | C |
| ATOM | 1971 | O   | GLN | A | 256 | 17.969 | 49.443 | 22.384 | 1.00 | 19.92 | O |
| ATOM | 1972 | CB  | GLN | A | 256 | 17.778 | 50.849 | 25.095 | 1.00 | 20.01 | C |
| ATOM | 1973 | CG  | GLN | A | 256 | 16.736 | 51.095 | 26.197 | 1.00 | 21.20 | C |
| ATOM | 1974 | CD  | GLN | A | 256 | 16.741 | 52.513 | 26.764 | 1.00 | 22.14 | C |
| ATOM | 1975 | OE1 | GLN | A | 256 | 15.711 | 53.195 | 26.741 | 1.00 | 23.01 | O |
| ATOM | 1976 | NE2 | GLN | A | 256 | 17.874 | 52.943 | 27.298 | 1.00 | 21.42 | N |
| ATOM | 1977 | N   | ASN | A | 257 | 19.845 | 48.716 | 23.385 | 1.00 | 19.66 | N |
| ATOM | 1978 | CA  | ASN | A | 257 | 20.580 | 48.485 | 22.155 | 1.00 | 20.07 | C |
| ATOM | 1979 | C   | ASN | A | 257 | 20.757 | 47.005 | 21.811 | 1.00 | 20.73 | C |
| ATOM | 1980 | O   | ASN | A | 257 | 21.416 | 46.694 | 20.823 | 1.00 | 20.96 | O |
| ATOM | 1981 | CB  | ASN | A | 257 | 21.969 | 49.100 | 22.232 | 1.00 | 19.17 | C |
| ATOM | 1982 | CG  | ASN | A | 257 | 21.941 | 50.550 | 22.635 | 1.00 | 20.82 | C |
| ATOM | 1983 | OD1 | ASN | A | 257 | 22.413 | 50.902 | 23.722 | 1.00 | 21.51 | O |
| ATOM | 1984 | ND2 | ASN | A | 257 | 21.396 | 51.407 | 21.763 | 1.00 | 16.92 | N |
| ATOM | 1985 | N   | VAL | A | 258 | 20.190 | 46.098 | 22.596 | 1.00 | 21.59 | N |
| ATOM | 1986 | CA  | VAL | A | 258 | 20.410 | 44.660 | 22.347 | 1.00 | 23.34 | C |
| ATOM | 1987 | C   | VAL | A | 258 | 19.671 | 44.172 | 21.112 | 1.00 | 23.85 | C |
| ATOM | 1988 | O   | VAL | A | 258 | 18.549 | 44.611 | 20.818 | 1.00 | 24.10 | O |
| ATOM | 1989 | CB  | VAL | A | 258 | 20.015 | 43.806 | 23.573 | 1.00 | 23.68 | C |
| ATOM | 1990 | CG1 | VAL | A | 258 | 18.507 | 43.720 | 23.685 | 1.00 | 24.12 | C |
| ATOM | 1991 | CG2 | VAL | A | 258 | 20.570 | 42.436 | 23.445 | 1.00 | 28.30 | C |
| ATOM | 1992 | N   | VAL | A | 259 | 20.314 | 43.286 | 20.360 | 1.00 | 24.47 | N |
| ATOM | 1993 | CA  | VAL | A | 259 | 19.705 | 42.721 | 19.154 | 1.00 | 24.91 | C |
| ATOM | 1994 | C   | VAL | A | 259 | 20.004 | 41.215 | 19.140 | 1.00 | 24.93 | C |
| ATOM | 1995 | O   | VAL | A | 259 | 21.152 | 40.829 | 19.119 | 1.00 | 25.32 | O |
| ATOM | 1996 | CB  | VAL | A | 259 | 20.281 | 43.362 | 17.895 | 1.00 | 24.88 | C |
| ATOM | 1997 | CG1 | VAL | A | 259 | 19.667 | 42.738 | 16.670 | 1.00 | 26.38 | C |
| ATOM | 1998 | CG2 | VAL | A | 259 | 20.051 | 44.869 | 17.909 | 1.00 | 24.83 | C |
| ATOM | 1999 | N   | GLY | A | 260 | 18.974 | 40.381 | 19.186 | 1.00 | 25.06 | N |
| ATOM | 2000 | CA  | GLY | A | 260 | 19.166 | 38.944 | 19.232 | 1.00 | 25.64 | C |
| ATOM | 2001 | C   | GLY | A | 260 | 19.076 | 38.221 | 17.887 | 1.00 | 25.42 | C |
| ATOM | 2002 | O   | GLY | A | 260 | 18.679 | 38.796 | 16.869 | 1.00 | 25.77 | O |
| ATOM | 2003 | N   | TYR | A | 261 | 19.497 | 36.965 | 17.907 | 1.00 | 25.04 | N |
| ATOM | 2004 | CA  | TYR | A | 261 | 19.380 | 36.049 | 16.792 | 1.00 | 25.30 | C |
| ATOM | 2005 | C   | TYR | A | 261 | 18.428 | 34.973 | 17.328 | 1.00 | 24.63 | C |
| ATOM | 2006 | O   | TYR | A | 261 | 18.676 | 34.417 | 18.392 | 1.00 | 24.77 | O |
| ATOM | 2007 | CB  | TYR | A | 261 | 20.729 | 35.414 | 16.482 | 1.00 | 25.84 | C |
| ATOM | 2008 | CG  | TYR | A | 261 | 21.750 | 36.315 | 15.825 | 1.00 | 28.57 | C |
| ATOM | 2009 | CD1 | TYR | A | 261 | 21.821 | 36.423 | 14.447 | 1.00 | 34.41 | C |
| ATOM | 2010 | CD2 | TYR | A | 261 | 22.631 | 37.049 | 16.574 | 1.00 | 29.87 | C |
| ATOM | 2011 | CE1 | TYR | A | 261 | 22.752 | 37.255 | 13.838 | 1.00 | 35.64 | C |
| ATOM | 2012 | CE2 | TYR | A | 261 | 23.576 | 37.852 | 15.986 | 1.00 | 32.26 | C |
| ATOM | 2013 | CZ  | TYR | A | 261 | 23.644 | 37.949 | 14.623 | 1.00 | 34.92 | C |
| ATOM | 2014 | OH  | TYR | A | 261 | 24.582 | 38.772 | 14.047 | 1.00 | 38.39 | O |
| ATOM | 2015 | N   | GLU | A | 262 | 17.325 | 34.698 | 16.658 | 1.00 | 23.64 | N |
| ATOM | 2016 | CA  | GLU | A | 262 | 16.376 | 33.758 | 17.244 | 1.00 | 24.03 | C |
| ATOM | 2017 | C   | GLU | A | 262 | 15.933 | 32.660 | 16.306 | 1.00 | 23.15 | C |
| ATOM | 2018 | O   | GLU | A | 262 | 16.063 | 32.766 | 15.078 | 1.00 | 22.51 | O |
| ATOM | 2019 | CB  | GLU | A | 262 | 15.172 | 34.482 | 17.861 | 1.00 | 24.11 | C |
| ATOM | 2020 | CG  | GLU | A | 262 | 13.899 | 34.502 | 17.057 | 1.00 | 26.35 | C |
| ATOM | 2021 | CD  | GLU | A | 262 | 12.744 | 35.177 | 17.785 | 1.00 | 27.98 | C |
| ATOM | 2022 | OE1 | GLU | A | 262 | 12.743 | 36.415 | 17.872 | 1.00 | 27.19 | O |
| ATOM | 2023 | OE2 | GLU | A | 262 | 11.818 | 34.476 | 18.254 | 1.00 | 29.21 | O |
| ATOM | 2024 | N   | THR | A | 263 | 15.455 | 31.587 | 16.917 | 1.00 | 22.58 | N |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2025 | CA  | THR | A | 263 | 14.939 | 30.458 | 16.170 | 1.00 | 22.52 | C |
| ATOM | 2026 | C   | THR | A | 263 | 14.047 | 29.617 | 17.076 | 1.00 | 22.48 | C |
| ATOM | 2027 | O   | THR | A | 263 | 14.107 | 29.712 | 18.313 | 1.00 | 22.14 | O |
| ATOM | 2028 | CB  | THR | A | 263 | 16.117 | 29.607 | 15.659 | 1.00 | 22.55 | C |
| ATOM | 2029 | OG1 | THR | A | 263 | 15.665 | 28.666 | 14.675 | 1.00 | 22.25 | O |
| ATOM | 2030 | CG2 | THR | A | 263 | 16.693 | 28.743 | 16.770 | 1.00 | 22.79 | C |
| ATOM | 2031 | N   | VAL | A | 264 | 13.208 | 28.797 | 16.472 | 1.00 | 21.62 | N |
| ATOM | 2032 | CA  | VAL | A | 264 | 12.453 | 27.860 | 17.263 | 1.00 | 22.45 | C |
| ATOM | 2033 | C   | VAL | A | 264 | 12.871 | 26.474 | 16.837 | 1.00 | 22.76 | C |
| ATOM | 2034 | O   | VAL | A | 264 | 12.779 | 26.134 | 15.673 | 1.00 | 22.77 | O |
| ATOM | 2035 | CB  | VAL | A | 264 | 10.964 | 28.027 | 17.087 | 1.00 | 23.08 | C |
| ATOM | 2036 | CG1 | VAL | A | 264 | 10.234 | 26.805 | 17.643 | 1.00 | 23.67 | C |
| ATOM | 2037 | CG2 | VAL | A | 264 | 10.499 | 29.344 | 17.767 | 1.00 | 22.75 | C |
| ATOM | 2038 | N   | VAL | A | 265 | 13.389 | 25.695 | 17.777 | 1.00 | 22.93 | N |
| ATOM | 2039 | CA  | VAL | A | 265 | 13.779 | 24.329 | 17.458 | 1.00 | 23.08 | C |
| ATOM | 2040 | C   | VAL | A | 265 | 12.738 | 23.317 | 17.886 | 1.00 | 22.86 | C |
| ATOM | 2041 | O   | VAL | A | 265 | 12.105 | 23.473 | 18.932 | 1.00 | 23.06 | O |
| ATOM | 2042 | CB  | VAL | A | 265 | 15.143 | 23.937 | 18.075 | 1.00 | 22.94 | C |
| ATOM | 2043 | CG1 | VAL | A | 265 | 16.243 | 24.745 | 17.404 | 1.00 | 23.66 | C |
| ATOM | 2044 | CG2 | VAL | A | 265 | 15.169 | 24.122 | 19.592 | 1.00 | 22.99 | C |
| ATOM | 2045 | N   | GLY | A | 266 | 12.574 | 22.290 | 17.056 | 1.00 | 21.77 | N |
| ATOM | 2046 | CA  | GLY | A | 266 | 11.683 | 21.178 | 17.355 | 1.00 | 21.98 | C |
| ATOM | 2047 | C   | GLY | A | 266 | 12.376 | 19.826 | 17.263 | 1.00 | 20.97 | C |
| ATOM | 2048 | O   | GLY | A | 266 | 13.562 | 19.757 | 16.999 | 1.00 | 20.63 | O |
| ATOM | 2049 | N   | PRO | A | 267 | 11.643 | 18.737 | 17.461 | 1.00 | 21.23 | N |
| ATOM | 2050 | CA  | PRO | A | 267 | 12.253 | 17.403 | 17.427 | 1.00 | 20.68 | C |
| ATOM | 2051 | C   | PRO | A | 267 | 13.126 | 17.183 | 16.203 | 1.00 | 20.04 | C |
| ATOM | 2052 | O   | PRO | A | 267 | 12.666 | 17.371 | 15.081 | 1.00 | 19.35 | O |
| ATOM | 2053 | CB  | PRO | A | 267 | 11.039 | 16.463 | 17.379 | 1.00 | 21.29 | C |
| ATOM | 2054 | CG  | PRO | A | 267 | 9.970  | 17.202 | 18.037 | 1.00 | 22.85 | C |
| ATOM | 2055 | CD  | PRO | A | 267 | 10.188 | 18.676 | 17.710 | 1.00 | 21.61 | C |
| ATOM | 2056 | N   | GLY | A | 268 | 14.376 | 16.787 | 16.411 | 1.00 | 20.31 | N |
| ATOM | 2057 | CA  | GLY | A | 268 | 15.278 | 16.518 | 15.305 | 1.00 | 19.95 | C |
| ATOM | 2058 | C   | GLY | A | 268 | 16.256 | 17.627 | 14.993 | 1.00 | 20.50 | C |
| ATOM | 2059 | O   | GLY | A | 268 | 17.277 | 17.400 | 14.311 | 1.00 | 21.62 | O |
| ATOM | 2060 | N   | ASP | A | 269 | 15.965 | 18.831 | 15.477 | 1.00 | 19.81 | N |
| ATOM | 2061 | CA  | ASP | A | 269 | 16.818 | 19.977 | 15.217 | 1.00 | 19.75 | C |
| ATOM | 2062 | C   | ASP | A | 269 | 17.970 | 20.003 | 16.215 | 1.00 | 19.67 | C |
| ATOM | 2063 | O   | ASP | A | 269 | 17.811 | 19.625 | 17.377 | 1.00 | 18.76 | O |
| ATOM | 2064 | CB  | ASP | A | 269 | 16.032 | 21.288 | 15.386 | 1.00 | 19.99 | C |
| ATOM | 2065 | CG  | ASP | A | 269 | 14.916 | 21.464 | 14.374 | 1.00 | 20.91 | C |
| ATOM | 2066 | OD1 | ASP | A | 269 | 14.935 | 20.842 | 13.287 | 1.00 | 22.13 | O |
| ATOM | 2067 | OD2 | ASP | A | 269 | 13.987 | 22.259 | 14.576 | 1.00 | 23.27 | O |
| ATOM | 2068 | N   | VAL | A | 270 | 19.116 | 20.481 | 15.746 | 1.00 | 19.56 | N |
| ATOM | 2069 | CA  | VAL | A | 270 | 20.276 | 20.700 | 16.595 | 1.00 | 19.57 | C |
| ATOM | 2070 | C   | VAL | A | 270 | 20.747 | 22.137 | 16.444 | 1.00 | 19.33 | C |
| ATOM | 2071 | O   | VAL | A | 270 | 21.033 | 22.594 | 15.352 | 1.00 | 19.78 | O |
| ATOM | 2072 | CB  | VAL | A | 270 | 21.404 | 19.776 | 16.215 | 1.00 | 19.55 | C |
| ATOM | 2073 | CG1 | VAL | A | 270 | 22.646 | 20.154 | 16.966 | 1.00 | 20.05 | C |
| ATOM | 2074 | CG2 | VAL | A | 270 | 21.001 | 18.342 | 16.535 | 1.00 | 19.44 | C |
| ATOM | 2075 | N   | LEU | A | 271 | 20.786 | 22.870 | 17.539 | 1.00 | 19.33 | N |
| ATOM | 2076 | CA  | LEU | A | 271 | 21.263 | 24.229 | 17.501 | 1.00 | 19.02 | C |
| ATOM | 2077 | C   | LEU | A | 271 | 22.677 | 24.272 | 18.036 | 1.00 | 19.15 | C |
| ATOM | 2078 | O   | LEU | A | 271 | 22.961 | 23.787 | 19.130 | 1.00 | 18.74 | O |
| ATOM | 2079 | CB  | LEU | A | 271 | 20.376 | 25.120 | 18.331 | 1.00 | 19.93 | C |
| ATOM | 2080 | CG  | LEU | A | 271 | 20.892 | 26.549 | 18.573 | 1.00 | 20.11 | C |
| ATOM | 2081 | CD1 | LEU | A | 271 | 21.011 | 27.358 | 17.296 | 1.00 | 19.41 | C |
| ATOM | 2082 | CD2 | LEU | A | 271 | 19.979 | 27.245 | 19.555 | 1.00 | 20.25 | C |
| ATOM | 2083 | N   | TYR | A | 272 | 23.582 | 24.818 | 17.244 | 1.00 | 19.15 | N |
| ATOM | 2084 | CA  | TYR | A | 272 | 24.924 | 25.051 | 17.718 | 1.00 | 19.70 | C |
| ATOM | 2085 | C   | TYR | A | 272 | 24.914 | 26.360 | 18.483 | 1.00 | 19.63 | C |

|      |      |     |           |        |        |        |      |       |   |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 2086 | O   | TYR A 272 | 24.646 | 27.395 | 17.897 | 1.00 | 20.44 | O |
| ATOM | 2087 | CB  | TYR A 272 | 25.908 | 25.172 | 16.547 | 1.00 | 19.86 | C |
| ATOM | 2088 | CG  | TYR A 272 | 27.293 | 25.654 | 16.962 | 1.00 | 21.59 | C |
| ATOM | 2089 | CD1 | TYR A 272 | 27.952 | 25.093 | 18.048 | 1.00 | 22.02 | C |
| ATOM | 2090 | CD2 | TYR A 272 | 27.936 | 26.668 | 16.278 | 1.00 | 20.87 | C |
| ATOM | 2091 | CE1 | TYR A 272 | 29.214 | 25.522 | 18.421 | 1.00 | 19.87 | C |
| ATOM | 2092 | CE2 | TYR A 272 | 29.200 | 27.098 | 16.649 | 1.00 | 20.88 | C |
| ATOM | 2093 | CZ  | TYR A 272 | 29.834 | 26.517 | 17.721 | 1.00 | 21.07 | C |
| ATOM | 2094 | OH  | TYR A 272 | 31.091 | 26.937 | 18.104 | 1.00 | 18.93 | O |
| ATOM | 2095 | N   | ILE A 273 | 25.210 | 26.308 | 19.776 | 1.00 | 19.80 | N |
| ATOM | 2096 | CA  | ILE A 273 | 25.342 | 27.500 | 20.598 | 1.00 | 20.12 | C |
| ATOM | 2097 | C   | ILE A 273 | 26.837 | 27.683 | 20.883 | 1.00 | 20.39 | C |
| ATOM | 2098 | O   | ILE A 273 | 27.393 | 27.000 | 21.760 | 1.00 | 19.88 | O |
| ATOM | 2099 | CB  | ILE A 273 | 24.576 | 27.366 | 21.901 | 1.00 | 19.72 | C |
| ATOM | 2100 | CG1 | ILE A 273 | 23.111 | 27.045 | 21.624 | 1.00 | 20.57 | C |
| ATOM | 2101 | CG2 | ILE A 273 | 24.661 | 28.695 | 22.696 | 1.00 | 20.99 | C |
| ATOM | 2102 | CD1 | ILE A 273 | 22.296 | 26.797 | 22.876 | 1.00 | 20.93 | C |
| ATOM | 2103 | N   | PRO A 274 | 27.487 | 28.611 | 20.182 | 1.00 | 20.23 | N |
| ATOM | 2104 | CA  | PRO A 274 | 28.938 | 28.743 | 20.326 | 1.00 | 21.16 | C |
| ATOM | 2105 | C   | PRO A 274 | 29.289 | 29.264 | 21.704 | 1.00 | 21.39 | C |
| ATOM | 2106 | O   | PRO A 274 | 28.520 | 30.027 | 22.317 | 1.00 | 20.89 | O |
| ATOM | 2107 | CB  | PRO A 274 | 29.353 | 29.757 | 19.230 | 1.00 | 21.62 | C |
| ATOM | 2108 | CG  | PRO A 274 | 28.089 | 30.056 | 18.410 | 1.00 | 21.22 | C |
| ATOM | 2109 | CD  | PRO A 274 | 26.919 | 29.621 | 19.282 | 1.00 | 20.51 | C |
| ATOM | 2110 | N   | MET A 275 | 30.450 | 28.831 | 22.180 | 1.00 | 21.53 | N |
| ATOM | 2111 | CA  | MET A 275 | 30.953 | 29.207 | 23.479 | 1.00 | 22.30 | C |
| ATOM | 2112 | C   | MET A 275 | 30.920 | 30.734 | 23.636 | 1.00 | 21.94 | C |
| ATOM | 2113 | O   | MET A 275 | 31.160 | 31.442 | 22.675 | 1.00 | 20.78 | O |
| ATOM | 2114 | CB  | MET A 275 | 32.367 | 28.695 | 23.589 | 1.00 | 23.06 | C |
| ATOM | 2115 | CG  | MET A 275 | 32.937 | 28.734 | 24.966 | 1.00 | 27.00 | C |
| ATOM | 2116 | SD  | MET A 275 | 34.545 | 27.926 | 24.991 | 1.00 | 33.74 | S |
| ATOM | 2117 | CE  | MET A 275 | 35.263 | 28.479 | 23.499 | 1.00 | 32.50 | C |
| ATOM | 2118 | N   | TYR A 276 | 30.583 | 31.211 | 24.832 | 1.00 | 21.96 | N |
| ATOM | 2119 | CA  | TYR A 276 | 30.485 | 32.656 | 25.138 | 1.00 | 23.15 | C |
| ATOM | 2120 | C   | TYR A 276 | 29.256 | 33.365 | 24.546 | 1.00 | 22.39 | C |
| ATOM | 2121 | O   | TYR A 276 | 28.989 | 34.496 | 24.899 | 1.00 | 22.58 | O |
| ATOM | 2122 | CB  | TYR A 276 | 31.776 | 33.409 | 24.760 | 1.00 | 23.80 | C |
| ATOM | 2123 | CG  | TYR A 276 | 32.904 | 33.136 | 25.729 | 1.00 | 28.82 | C |
| ATOM | 2124 | CD1 | TYR A 276 | 32.940 | 33.756 | 26.951 | 1.00 | 32.73 | C |
| ATOM | 2125 | CD2 | TYR A 276 | 33.935 | 32.246 | 25.415 | 1.00 | 35.83 | C |
| ATOM | 2126 | CE1 | TYR A 276 | 33.956 | 33.507 | 27.864 | 1.00 | 35.96 | C |
| ATOM | 2127 | CE2 | TYR A 276 | 34.975 | 31.992 | 26.336 | 1.00 | 38.59 | C |
| ATOM | 2128 | CZ  | TYR A 276 | 34.958 | 32.628 | 27.562 | 1.00 | 38.60 | C |
| ATOM | 2129 | OH  | TYR A 276 | 35.951 | 32.421 | 28.513 | 1.00 | 45.18 | O |
| ATOM | 2130 | N   | TRP A 277 | 28.488 | 32.709 | 23.684 | 1.00 | 21.71 | N |
| ATOM | 2131 | CA  | TRP A 277 | 27.281 | 33.350 | 23.149 | 1.00 | 21.24 | C |
| ATOM | 2132 | C   | TRP A 277 | 26.184 | 33.278 | 24.152 | 1.00 | 20.90 | C |
| ATOM | 2133 | O   | TRP A 277 | 25.914 | 32.217 | 24.708 | 1.00 | 21.96 | O |
| ATOM | 2134 | CB  | TRP A 277 | 26.790 | 32.711 | 21.856 | 1.00 | 21.01 | C |
| ATOM | 2135 | CG  | TRP A 277 | 27.547 | 33.166 | 20.670 | 1.00 | 19.98 | C |
| ATOM | 2136 | CD1 | TRP A 277 | 28.875 | 33.013 | 20.462 | 1.00 | 17.90 | C |
| ATOM | 2137 | CD2 | TRP A 277 | 27.030 | 33.832 | 19.519 | 1.00 | 19.76 | C |
| ATOM | 2138 | NE1 | TRP A 277 | 29.218 | 33.533 | 19.247 | 1.00 | 18.64 | N |
| ATOM | 2139 | CE2 | TRP A 277 | 28.106 | 34.071 | 18.662 | 1.00 | 18.29 | C |
| ATOM | 2140 | CE3 | TRP A 277 | 25.764 | 34.305 | 19.151 | 1.00 | 20.56 | C |
| ATOM | 2141 | CZ2 | TRP A 277 | 27.963 | 34.716 | 17.442 | 1.00 | 19.63 | C |
| ATOM | 2142 | CZ3 | TRP A 277 | 25.624 | 34.950 | 17.943 | 1.00 | 21.16 | C |
| ATOM | 2143 | CH2 | TRP A 277 | 26.720 | 35.137 | 17.095 | 1.00 | 19.92 | C |
| ATOM | 2144 | N   | TRP A 278 | 25.574 | 34.426 | 24.405 | 1.00 | 20.32 | N |
| ATOM | 2145 | CA  | TRP A 278 | 24.452 | 34.533 | 25.316 | 1.00 | 20.13 | C |
| ATOM | 2146 | C   | TRP A 278 | 23.268 | 33.787 | 24.741 | 1.00 | 19.99 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2147 | O   | TRP | A | 278 | 23.083 | 33.758 | 23.538 | 1.00 | 20.42 | O |
| ATOM | 2148 | CB  | TRP | A | 278 | 24.025 | 35.999 | 25.441 | 1.00 | 20.65 | C |
| ATOM | 2149 | CG  | TRP | A | 278 | 25.031 | 36.864 | 26.107 | 1.00 | 20.56 | C |
| ATOM | 2150 | CD1 | TRP | A | 278 | 26.078 | 37.526 | 25.519 | 1.00 | 19.63 | C |
| ATOM | 2151 | CD2 | TRP | A | 278 | 25.096 | 37.160 | 27.501 | 1.00 | 19.59 | C |
| ATOM | 2152 | NE1 | TRP | A | 278 | 26.772 | 38.233 | 26.469 | 1.00 | 20.70 | N |
| ATOM | 2153 | CE2 | TRP | A | 278 | 26.191 | 38.012 | 27.699 | 1.00 | 20.10 | C |
| ATOM | 2154 | CE3 | TRP | A | 278 | 24.318 | 36.811 | 28.601 | 1.00 | 20.98 | C |
| ATOM | 2155 | CZ2 | TRP | A | 278 | 26.527 | 38.516 | 28.951 | 1.00 | 20.24 | C |
| ATOM | 2156 | CZ3 | TRP | A | 278 | 24.668 | 37.299 | 29.849 | 1.00 | 23.26 | C |
| ATOM | 2157 | CH2 | TRP | A | 278 | 25.759 | 38.146 | 30.011 | 1.00 | 20.41 | C |
| ATOM | 2158 | N   | HIS | A | 279 | 22.463 | 33.194 | 25.591 | 1.00 | 19.84 | N |
| ATOM | 2159 | CA  | HIS | A | 279 | 21.269 | 32.530 | 25.122 | 1.00 | 20.78 | C |
| ATOM | 2160 | C   | HIS | A | 279 | 20.202 | 32.495 | 26.192 | 1.00 | 20.37 | C |
| ATOM | 2161 | O   | HIS | A | 279 | 20.479 | 32.275 | 27.370 | 1.00 | 20.66 | O |
| ATOM | 2162 | CB  | HIS | A | 279 | 21.540 | 31.098 | 24.604 | 1.00 | 20.86 | C |
| ATOM | 2163 | CG  | HIS | A | 279 | 22.349 | 30.238 | 25.528 | 1.00 | 21.83 | C |
| ATOM | 2164 | ND1 | HIS | A | 279 | 23.720 | 30.324 | 25.608 | 1.00 | 23.19 | N |
| ATOM | 2165 | CD2 | HIS | A | 279 | 21.988 | 29.240 | 26.371 | 1.00 | 23.96 | C |
| ATOM | 2166 | CE1 | HIS | A | 279 | 24.175 | 29.411 | 26.449 | 1.00 | 22.20 | C |
| ATOM | 2167 | NE2 | HIS | A | 279 | 23.144 | 28.747 | 26.940 | 1.00 | 23.84 | N |
| ATOM | 2168 | N   | HIS | A | 280 | 18.994 | 32.718 | 25.711 | 1.00 | 20.90 | N |
| ATOM | 2169 | CA  | HIS | A | 280 | 17.742 | 32.758 | 26.441 | 1.00 | 21.22 | C |
| ATOM | 2170 | C   | HIS | A | 280 | 16.910 | 31.676 | 25.793 | 1.00 | 21.42 | C |
| ATOM | 2171 | O   | HIS | A | 280 | 16.749 | 31.685 | 24.580 | 1.00 | 21.70 | O |
| ATOM | 2172 | CB  | HIS | A | 280 | 17.099 | 34.124 | 26.224 | 1.00 | 21.04 | C |
| ATOM | 2173 | CG  | HIS | A | 280 | 15.632 | 34.168 | 26.489 | 1.00 | 21.54 | C |
| ATOM | 2174 | ND1 | HIS | A | 280 | 15.096 | 34.836 | 27.571 | 1.00 | 22.76 | N |
| ATOM | 2175 | CD2 | HIS | A | 280 | 14.581 | 33.660 | 25.802 | 1.00 | 22.74 | C |
| ATOM | 2176 | CE1 | HIS | A | 280 | 13.779 | 34.721 | 27.546 | 1.00 | 23.23 | C |
| ATOM | 2177 | NE2 | HIS | A | 280 | 13.441 | 34.014 | 26.482 | 1.00 | 23.05 | N |
| ATOM | 2178 | N   | ILE | A | 281 | 16.367 | 30.755 | 26.584 | 1.00 | 22.31 | N |
| ATOM | 2179 | CA  | ILE | A | 281 | 15.649 | 29.599 | 26.040 | 1.00 | 22.39 | C |
| ATOM | 2180 | C   | ILE | A | 281 | 14.304 | 29.443 | 26.722 | 1.00 | 22.72 | C |
| ATOM | 2181 | O   | ILE | A | 281 | 14.216 | 29.419 | 27.945 | 1.00 | 22.70 | O |
| ATOM | 2182 | CB  | ILE | A | 281 | 16.527 | 28.336 | 26.189 | 1.00 | 22.98 | C |
| ATOM | 2183 | CG1 | ILE | A | 281 | 17.771 | 28.504 | 25.305 | 1.00 | 24.90 | C |
| ATOM | 2184 | CG2 | ILE | A | 281 | 15.770 | 27.059 | 25.771 | 1.00 | 21.60 | C |
| ATOM | 2185 | CD1 | ILE | A | 281 | 18.795 | 27.556 | 25.554 | 1.00 | 27.31 | C |
| ATOM | 2186 | N   | GLU | A | 282 | 13.252 | 29.350 | 25.920 | 1.00 | 22.93 | N |
| ATOM | 2187 | CA  | GLU | A | 282 | 11.903 | 29.205 | 26.458 | 1.00 | 23.35 | C |
| ATOM | 2188 | C   | GLU | A | 282 | 11.101 | 28.105 | 25.769 | 1.00 | 22.59 | C |
| ATOM | 2189 | O   | GLU | A | 282 | 11.092 | 27.982 | 24.549 | 1.00 | 21.77 | O |
| ATOM | 2190 | CB  | GLU | A | 282 | 11.144 | 30.538 | 26.393 | 1.00 | 23.47 | C |
| ATOM | 2191 | CG  | GLU | A | 282 | 10.830 | 31.055 | 25.009 | 1.00 | 25.70 | C |
| ATOM | 2192 | CD  | GLU | A | 282 | 10.281 | 32.483 | 25.023 | 1.00 | 25.79 | C |
| ATOM | 2193 | OE1 | GLU | A | 282 | 10.898 | 33.356 | 25.665 | 1.00 | 27.49 | O |
| ATOM | 2194 | OE2 | GLU | A | 282 | 9.241  | 32.740 | 24.391 | 1.00 | 26.03 | O |
| ATOM | 2195 | N   | SER | A | 283 | 10.456 | 27.293 | 26.588 | 1.00 | 22.44 | N |
| ATOM | 2196 | CA  | SER | A | 283 | 9.570  | 26.246 | 26.103 | 1.00 | 23.00 | C |
| ATOM | 2197 | C   | SER | A | 283 | 8.256  | 26.916 | 25.753 | 1.00 | 23.56 | C |
| ATOM | 2198 | O   | SER | A | 283 | 7.685  | 27.615 | 26.584 | 1.00 | 24.14 | O |
| ATOM | 2199 | CB  | SER | A | 283 | 9.346  | 25.204 | 27.188 | 1.00 | 22.59 | C |
| ATOM | 2200 | OG  | SER | A | 283 | 10.496 | 24.400 | 27.345 | 1.00 | 22.67 | O |
| ATOM | 2201 | N   | LEU | A | 284 | 7.763  | 26.694 | 24.541 | 1.00 | 24.07 | N |
| ATOM | 2202 | CA  | LEU | A | 284 | 6.581  | 27.412 | 24.070 | 1.00 | 24.80 | C |
| ATOM | 2203 | C   | LEU | A | 284 | 5.386  | 27.324 | 25.004 | 1.00 | 24.51 | C |
| ATOM | 2204 | O   | LEU | A | 284 | 5.098  | 26.271 | 25.602 | 1.00 | 23.93 | O |
| ATOM | 2205 | CB  | LEU | A | 284 | 6.161  | 26.947 | 22.682 | 1.00 | 25.09 | C |
| ATOM | 2206 | CG  | LEU | A | 284 | 7.185  | 27.083 | 21.555 | 1.00 | 26.46 | C |
| ATOM | 2207 | CD1 | LEU | A | 284 | 6.475  | 27.236 | 20.215 | 1.00 | 28.29 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2208 | CD2 | LEU | A | 284 | 8.123  | 28.188 | 21.775 | 1.00 | 26.10 | C |
| ATOM | 2209 | N   | LEU | A | 285 | 4.718  | 28.463 | 25.136 | 1.00 | 24.41 | N |
| ATOM | 2210 | CA  | LEU | A | 285 | 3.506  | 28.554 | 25.930 | 1.00 | 24.83 | C |
| ATOM | 2211 | C   | LEU | A | 285 | 2.526  | 27.583 | 25.323 | 1.00 | 24.68 | C |
| ATOM | 2212 | O   | LEU | A | 285 | 2.393  | 27.516 | 24.110 | 1.00 | 24.08 | O |
| ATOM | 2213 | CB  | LEU | A | 285 | 2.927  | 29.961 | 25.872 | 1.00 | 24.79 | C |
| ATOM | 2214 | CG  | LEU | A | 285 | 3.825  | 31.078 | 26.397 | 1.00 | 25.19 | C |
| ATOM | 2215 | CD1 | LEU | A | 285 | 3.298  | 32.434 | 25.954 | 1.00 | 26.02 | C |
| ATOM | 2216 | CD2 | LEU | A | 285 | 3.925  | 30.999 | 27.898 | 1.00 | 26.27 | C |
| ATOM | 2217 | N   | ASN | A | 286 | 1.867  | 26.815 | 26.173 | 1.00 | 25.20 | N |
| ATOM | 2218 | CA  | ASN | A | 286 | 0.867  | 25.848 | 25.730 | 1.00 | 25.85 | C |
| ATOM | 2219 | C   | ASN | A | 286 | 1.371  | 24.791 | 24.742 | 1.00 | 25.23 | C |
| ATOM | 2220 | O   | ASN | A | 286 | 0.594  | 24.267 | 23.965 | 1.00 | 24.38 | O |
| ATOM | 2221 | CB  | ASN | A | 286 | -0.319 | 26.599 | 25.124 | 1.00 | 26.54 | C |
| ATOM | 2222 | CG  | ASN | A | 286 | -0.957 | 27.546 | 26.109 | 1.00 | 29.40 | C |
| ATOM | 2223 | OD1 | ASN | A | 286 | -1.478 | 27.118 | 27.140 | 1.00 | 33.49 | O |
| ATOM | 2224 | ND2 | ASN | A | 286 | -0.893 | 28.843 | 25.821 | 1.00 | 33.58 | N |
| ATOM | 2225 | N   | GLY | A | 287 | 2.669  | 24.487 | 24.774 | 1.00 | 24.55 | N |
| ATOM | 2226 | CA  | GLY | A | 287 | 3.243  | 23.518 | 23.863 | 1.00 | 24.10 | C |
| ATOM | 2227 | C   | GLY | A | 287 | 3.524  | 22.167 | 24.487 | 1.00 | 23.80 | C |
| ATOM | 2228 | O   | GLY | A | 287 | 4.110  | 21.301 | 23.838 | 1.00 | 24.10 | O |
| ATOM | 2229 | N   | GLY | A | 288 | 3.100  | 21.971 | 25.734 | 1.00 | 23.32 | N |
| ATOM | 2230 | CA  | GLY | A | 288 | 3.360  | 20.730 | 26.439 | 1.00 | 23.24 | C |
| ATOM | 2231 | C   | GLY | A | 288 | 4.808  | 20.673 | 26.903 | 1.00 | 23.49 | C |
| ATOM | 2232 | O   | GLY | A | 288 | 5.548  | 21.646 | 26.741 | 1.00 | 22.86 | O |
| ATOM | 2233 | N   | ILE | A | 289 | 5.220  | 19.539 | 27.462 | 1.00 | 23.36 | N |
| ATOM | 2234 | CA  | ILE | A | 289 | 6.571  | 19.406 | 27.983 | 1.00 | 23.99 | C |
| ATOM | 2235 | C   | ILE | A | 289 | 7.601  | 19.374 | 26.874 | 1.00 | 23.28 | C |
| ATOM | 2236 | O   | ILE | A | 289 | 7.324  | 18.958 | 25.755 | 1.00 | 23.68 | O |
| ATOM | 2237 | CB  | ILE | A | 289 | 6.750  | 18.123 | 28.817 | 1.00 | 24.68 | C |
| ATOM | 2238 | CG1 | ILE | A | 289 | 6.819  | 16.912 | 27.901 | 1.00 | 26.90 | C |
| ATOM | 2239 | CG2 | ILE | A | 289 | 5.648  | 17.983 | 29.885 | 1.00 | 25.75 | C |
| ATOM | 2240 | CD1 | ILE | A | 289 | 7.294  | 15.640 | 28.613 | 1.00 | 29.37 | C |
| ATOM | 2241 | N   | THR | A | 290 | 8.811  | 19.790 | 27.210 | 1.00 | 22.42 | N |
| ATOM | 2242 | CA  | THR | A | 290 | 9.904  | 19.768 | 26.264 | 1.00 | 21.38 | C |
| ATOM | 2243 | C   | THR | A | 290 | 11.030 | 18.880 | 26.774 | 1.00 | 20.56 | C |
| ATOM | 2244 | O   | THR | A | 290 | 11.243 | 18.743 | 27.986 | 1.00 | 19.81 | O |
| ATOM | 2245 | CB  | THR | A | 290 | 10.461 | 21.175 | 26.053 | 1.00 | 21.70 | C |
| ATOM | 2246 | OG1 | THR | A | 290 | 10.823 | 21.761 | 27.308 | 1.00 | 20.15 | O |
| ATOM | 2247 | CG2 | THR | A | 290 | 9.405  | 22.108 | 25.460 | 1.00 | 21.76 | C |
| ATOM | 2248 | N   | ILE | A | 291 | 11.757 | 18.296 | 25.841 | 1.00 | 19.36 | N |
| ATOM | 2249 | CA  | ILE | A | 291 | 12.903 | 17.503 | 26.190 | 1.00 | 19.73 | C |
| ATOM | 2250 | C   | ILE | A | 291 | 14.044 | 17.865 | 25.286 | 1.00 | 19.29 | C |
| ATOM | 2251 | O   | ILE | A | 291 | 13.862 | 17.976 | 24.083 | 1.00 | 19.81 | O |
| ATOM | 2252 | CB  | ILE | A | 291 | 12.598 | 15.992 | 26.085 | 1.00 | 20.08 | C |
| ATOM | 2253 | CG1 | ILE | A | 291 | 11.467 | 15.609 | 27.044 | 1.00 | 20.06 | C |
| ATOM | 2254 | CG2 | ILE | A | 291 | 13.873 | 15.214 | 26.378 | 1.00 | 20.21 | C |
| ATOM | 2255 | CD1 | ILE | A | 291 | 11.028 | 14.131 | 26.931 | 1.00 | 21.77 | C |
| ATOM | 2256 | N   | THR | A | 292 | 15.215 | 18.070 | 25.882 | 1.00 | 18.95 | N |
| ATOM | 2257 | CA  | THR | A | 292 | 16.406 | 18.407 | 25.156 | 1.00 | 19.17 | C |
| ATOM | 2258 | C   | THR | A | 292 | 17.589 | 17.691 | 25.753 | 1.00 | 19.18 | C |
| ATOM | 2259 | O   | THR | A | 292 | 17.671 | 17.497 | 26.965 | 1.00 | 19.21 | O |
| ATOM | 2260 | CB  | THR | A | 292 | 16.703 | 19.937 | 25.259 | 1.00 | 19.83 | C |
| ATOM | 2261 | OG1 | THR | A | 292 | 15.559 | 20.724 | 24.879 | 1.00 | 20.23 | O |
| ATOM | 2262 | CG2 | THR | A | 292 | 17.787 | 20.350 | 24.270 | 1.00 | 20.15 | C |
| ATOM | 2263 | N   | VAL | A | 293 | 18.530 | 17.314 | 24.903 | 1.00 | 19.25 | N |
| ATOM | 2264 | CA  | VAL | A | 293 | 19.809 | 16.824 | 25.387 | 1.00 | 19.51 | C |
| ATOM | 2265 | C   | VAL | A | 293 | 20.912 | 17.667 | 24.749 | 1.00 | 19.58 | C |
| ATOM | 2266 | O   | VAL | A | 293 | 20.962 | 17.792 | 23.535 | 1.00 | 18.47 | O |
| ATOM | 2267 | CB  | VAL | A | 293 | 20.024 | 15.345 | 25.063 | 1.00 | 19.73 | C |
| ATOM | 2268 | CG1 | VAL | A | 293 | 21.490 | 14.951 | 25.250 | 1.00 | 20.24 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2269 | CG2 | VAL | A | 293 | 19.146 | 14.478 | 25.968 | 1.00 | 20.65 | C |
| ATOM | 2270 | N   | ASN | A | 294 | 21.766 | 18.277 | 25.569 | 1.00 | 19.85 | N |
| ATOM | 2271 | CA  | ASN | A | 294 | 22.882 | 19.057 | 25.039 | 1.00 | 20.26 | C |
| ATOM | 2272 | C   | ASN | A | 294 | 24.179 | 18.232 | 25.052 | 1.00 | 20.35 | C |
| ATOM | 2273 | O   | ASN | A | 294 | 24.233 | 17.131 | 25.634 | 1.00 | 21.82 | O |
| ATOM | 2274 | CB  | ASN | A | 294 | 23.008 | 20.443 | 25.727 | 1.00 | 20.82 | C |
| ATOM | 2275 | CG  | ASN | A | 294 | 23.676 | 20.388 | 27.102 | 1.00 | 21.84 | C |
| ATOM | 2276 | OD1 | ASN | A | 294 | 24.209 | 19.354 | 27.495 | 1.00 | 21.66 | O |
| ATOM | 2277 | ND2 | ASN | A | 294 | 23.630 | 21.519 | 27.849 | 1.00 | 21.23 | N |
| ATOM | 2278 | N   | PHE | A | 295 | 25.186 | 18.729 | 24.346 | 1.00 | 20.69 | N |
| ATOM | 2279 | CA  | PHE | A | 295 | 26.490 | 18.095 | 24.233 | 1.00 | 20.46 | C |
| ATOM | 2280 | C   | PHE | A | 295 | 27.452 | 19.240 | 24.494 | 1.00 | 21.42 | C |
| ATOM | 2281 | O   | PHE | A | 295 | 27.573 | 20.167 | 23.653 | 1.00 | 20.85 | O |
| ATOM | 2282 | CB  | PHE | A | 295 | 26.728 | 17.569 | 22.814 | 1.00 | 20.62 | C |
| ATOM | 2283 | CG  | PHE | A | 295 | 25.898 | 16.366 | 22.440 | 1.00 | 21.15 | C |
| ATOM | 2284 | CD1 | PHE | A | 295 | 24.526 | 16.468 | 22.247 | 1.00 | 21.98 | C |
| ATOM | 2285 | CD2 | PHE | A | 295 | 26.498 | 15.130 | 22.256 | 1.00 | 19.31 | C |
| ATOM | 2286 | CE1 | PHE | A | 295 | 23.791 | 15.343 | 21.902 | 1.00 | 19.77 | C |
| ATOM | 2287 | CE2 | PHE | A | 295 | 25.762 | 14.037 | 21.885 | 1.00 | 17.96 | C |
| ATOM | 2288 | CZ  | PHE | A | 295 | 24.424 | 14.138 | 21.720 | 1.00 | 17.87 | C |
| ATOM | 2289 | N   | TRP | A | 296 | 28.123 | 19.196 | 25.645 | 1.00 | 21.19 | N |
| ATOM | 2290 | CA  | TRP | A | 296 | 29.023 | 20.275 | 26.050 | 1.00 | 21.46 | C |
| ATOM | 2291 | C   | TRP | A | 296 | 30.481 | 19.834 | 25.873 | 1.00 | 21.42 | C |
| ATOM | 2292 | O   | TRP | A | 296 | 30.898 | 18.795 | 26.387 | 1.00 | 21.96 | O |
| ATOM | 2293 | CB  | TRP | A | 296 | 28.760 | 20.669 | 27.498 | 1.00 | 21.13 | C |
| ATOM | 2294 | CG  | TRP | A | 296 | 27.853 | 21.859 | 27.710 | 1.00 | 21.95 | C |
| ATOM | 2295 | CD1 | TRP | A | 296 | 27.797 | 22.987 | 26.955 | 1.00 | 23.23 | C |
| ATOM | 2296 | CD2 | TRP | A | 296 | 26.935 | 22.067 | 28.797 | 1.00 | 22.27 | C |
| ATOM | 2297 | NE1 | TRP | A | 296 | 26.882 | 23.869 | 27.478 | 1.00 | 22.26 | N |
| ATOM | 2298 | CE2 | TRP | A | 296 | 26.336 | 23.329 | 28.607 | 1.00 | 22.53 | C |
| ATOM | 2299 | CE3 | TRP | A | 296 | 26.531 | 21.298 | 29.894 | 1.00 | 24.83 | C |
| ATOM | 2300 | CZ2 | TRP | A | 296 | 25.362 | 23.840 | 29.463 | 1.00 | 22.34 | C |
| ATOM | 2301 | CZ3 | TRP | A | 296 | 25.557 | 21.810 | 30.754 | 1.00 | 24.59 | C |
| ATOM | 2302 | CH2 | TRP | A | 296 | 24.993 | 23.075 | 30.531 | 1.00 | 23.75 | C |
| ATOM | 2303 | N   | TYR | A | 297 | 31.235 | 20.632 | 25.126 | 1.00 | 21.64 | N |
| ATOM | 2304 | CA  | TYR | A | 297 | 32.633 | 20.361 | 24.845 | 1.00 | 21.81 | C |
| ATOM | 2305 | C   | TYR | A | 297 | 33.482 | 21.523 | 25.320 | 1.00 | 22.41 | C |
| ATOM | 2306 | O   | TYR | A | 297 | 33.110 | 22.682 | 25.146 | 1.00 | 21.78 | O |
| ATOM | 2307 | CB  | TYR | A | 297 | 32.862 | 20.198 | 23.344 | 1.00 | 21.49 | C |
| ATOM | 2308 | CG  | TYR | A | 297 | 32.287 | 18.943 | 22.761 | 1.00 | 21.77 | C |
| ATOM | 2309 | CD1 | TYR | A | 297 | 30.934 | 18.870 | 22.415 | 1.00 | 21.68 | C |
| ATOM | 2310 | CD2 | TYR | A | 297 | 33.083 | 17.841 | 22.526 | 1.00 | 19.80 | C |
| ATOM | 2311 | CE1 | TYR | A | 297 | 30.405 | 17.734 | 21.890 | 1.00 | 22.16 | C |
| ATOM | 2312 | CE2 | TYR | A | 297 | 32.555 | 16.690 | 21.993 | 1.00 | 20.99 | C |
| ATOM | 2313 | CZ  | TYR | A | 297 | 31.215 | 16.637 | 21.686 | 1.00 | 21.46 | C |
| ATOM | 2314 | OH  | TYR | A | 297 | 30.673 | 15.494 | 21.159 | 1.00 | 22.11 | O |
| ATOM | 2315 | N   | LYS | A | 298 | 34.632 | 21.220 | 25.899 | 1.00 | 23.17 | N |
| ATOM | 2316 | CA  | LYS | A | 298 | 35.566 | 22.273 | 26.288 | 1.00 | 24.45 | C |
| ATOM | 2317 | C   | LYS | A | 298 | 36.074 | 22.912 | 25.021 | 1.00 | 24.21 | C |
| ATOM | 2318 | O   | LYS | A | 298 | 36.264 | 22.228 | 24.025 | 1.00 | 23.35 | O |
| ATOM | 2319 | CB  | LYS | A | 298 | 36.748 | 21.699 | 27.085 | 1.00 | 24.85 | C |
| ATOM | 2320 | CG  | LYS | A | 298 | 36.436 | 21.416 | 28.552 | 1.00 | 28.00 | C |
| ATOM | 2321 | CD  | LYS | A | 298 | 37.657 | 20.865 | 29.298 | 1.00 | 31.59 | C |
| ATOM | 2322 | CE  | LYS | A | 298 | 37.309 | 20.447 | 30.730 | 1.00 | 33.77 | C |
| ATOM | 2323 | NZ  | LYS | A | 298 | 38.406 | 19.627 | 31.367 | 1.00 | 36.02 | N |
| ATOM | 2324 | N   | GLY | A | 299 | 36.317 | 24.216 | 25.056 | 1.00 | 25.28 | N |
| ATOM | 2325 | CA  | GLY | A | 299 | 36.818 | 24.909 | 23.886 | 1.00 | 26.38 | C |
| ATOM | 2326 | C   | GLY | A | 299 | 38.254 | 24.542 | 23.547 | 1.00 | 27.78 | C |
| ATOM | 2327 | O   | GLY | A | 299 | 38.935 | 23.895 | 24.315 | 1.00 | 27.16 | O |
| ATOM | 2328 | N   | ALA | A | 300 | 38.690 | 24.949 | 22.366 | 1.00 | 30.42 | N |
| ATOM | 2329 | CA  | ALA | A | 300 | 40.062 | 24.762 | 21.918 | 1.00 | 32.93 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2330 | C   | ALA | A | 300 | 41.021 | 25.544 | 22.819 | 1.00 | 35.12 | C |
| ATOM | 2331 | O   | ALA | A | 300 | 40.597 | 26.337 | 23.646 | 1.00 | 34.87 | O |
| ATOM | 2332 | CB  | ALA | A | 300 | 40.199 | 25.249 | 20.472 | 1.00 | 32.98 | C |
| ATOM | 2333 | N   | PRO | A | 301 | 42.318 | 25.355 | 22.615 | 1.00 | 38.54 | N |
| ATOM | 2334 | CA  | PRO | A | 301 | 43.347 | 26.012 | 23.440 | 1.00 | 40.37 | C |
| ATOM | 2335 | C   | PRO | A | 301 | 43.548 | 27.484 | 23.102 | 1.00 | 41.99 | C |
| ATOM | 2336 | O   | PRO | A | 301 | 43.379 | 27.853 | 21.950 | 1.00 | 42.88 | O |
| ATOM | 2337 | CB  | PRO | A | 301 | 44.615 | 25.246 | 23.061 | 1.00 | 40.42 | C |
| ATOM | 2338 | CG  | PRO | A | 301 | 44.397 | 24.879 | 21.638 | 1.00 | 39.87 | C |
| ATOM | 2339 | CD  | PRO | A | 301 | 42.919 | 24.544 | 21.535 | 1.00 | 38.98 | C |
| ATOM | 2340 | N   | THR | A | 302 | 43.915 | 28.293 | 24.090 | 1.00 | 44.60 | N |
| ATOM | 2341 | CA  | THR | A | 302 | 44.209 | 29.725 | 23.912 | 1.00 | 46.30 | C |
| ATOM | 2342 | C   | THR | A | 302 | 45.593 | 29.790 | 23.315 | 1.00 | 47.41 | C |
| ATOM | 2343 | O   | THR | A | 302 | 46.534 | 29.388 | 23.992 | 1.00 | 47.96 | O |
| ATOM | 2344 | CB  | THR | A | 302 | 44.242 | 30.391 | 25.294 | 1.00 | 46.57 | C |
| ATOM | 2345 | OG1 | THR | A | 302 | 42.941 | 30.320 | 25.895 | 1.00 | 48.00 | O |
| ATOM | 2346 | CG2 | THR | A | 302 | 44.526 | 31.869 | 25.199 | 1.00 | 47.24 | C |
| ATOM | 2347 | N   | PRO | A | 303 | 45.782 | 30.336 | 22.112 | 1.00 | 48.55 | N |
| ATOM | 2348 | CA  | PRO | A | 303 | 47.090 | 30.170 | 21.473 | 1.00 | 48.80 | C |
| ATOM | 2349 | C   | PRO | A | 303 | 48.210 | 30.717 | 22.341 | 1.00 | 48.76 | C |
| ATOM | 2350 | O   | PRO | A | 303 | 47.874 | 31.450 | 23.269 | 1.00 | 49.07 | O |
| ATOM | 2351 | CB  | PRO | A | 303 | 46.967 | 30.980 | 20.185 | 1.00 | 49.07 | C |
| ATOM | 2352 | CG  | PRO | A | 303 | 45.504 | 31.101 | 19.952 | 1.00 | 48.93 | C |
| ATOM | 2353 | CD  | PRO | A | 303 | 44.916 | 31.243 | 21.330 | 1.00 | 48.62 | C |
| ATOM | 2354 | N   | GLU | A | 307 | 46.795 | 36.776 | 18.436 | 1.00 | 52.62 | N |
| ATOM | 2355 | CA  | GLU | A | 307 | 46.885 | 37.814 | 17.415 | 1.00 | 52.76 | C |
| ATOM | 2356 | C   | GLU | A | 307 | 45.865 | 38.906 | 17.636 | 1.00 | 52.00 | C |
| ATOM | 2357 | O   | GLU | A | 307 | 44.757 | 38.658 | 18.096 | 1.00 | 52.48 | O |
| ATOM | 2358 | CB  | GLU | A | 307 | 46.686 | 37.246 | 15.996 | 1.00 | 53.32 | C |
| ATOM | 2359 | CG  | GLU | A | 307 | 46.893 | 38.307 | 14.908 | 1.00 | 54.63 | C |
| ATOM | 2360 | CD  | GLU | A | 307 | 46.862 | 37.764 | 13.487 | 1.00 | 56.43 | C |
| ATOM | 2361 | OE1 | GLU | A | 307 | 46.527 | 36.574 | 13.290 | 1.00 | 57.49 | O |
| ATOM | 2362 | OE2 | GLU | A | 307 | 47.173 | 38.543 | 12.558 | 1.00 | 57.89 | O |
| ATOM | 2363 | N   | TYR | A | 308 | 46.255 | 40.125 | 17.303 | 1.00 | 51.19 | N |
| ATOM | 2364 | CA  | TYR | A | 308 | 45.367 | 41.267 | 17.405 | 1.00 | 50.55 | C |
| ATOM | 2365 | C   | TYR | A | 308 | 44.747 | 41.494 | 16.039 | 1.00 | 49.51 | C |
| ATOM | 2366 | O   | TYR | A | 308 | 45.300 | 41.053 | 15.028 | 1.00 | 49.70 | O |
| ATOM | 2367 | CB  | TYR | A | 308 | 46.151 | 42.485 | 17.867 | 1.00 | 50.82 | C |
| ATOM | 2368 | CG  | TYR | A | 308 | 46.702 | 42.286 | 19.259 | 1.00 | 52.47 | C |
| ATOM | 2369 | CD1 | TYR | A | 308 | 45.949 | 42.632 | 20.373 | 1.00 | 53.15 | C |
| ATOM | 2370 | CD2 | TYR | A | 308 | 47.948 | 41.696 | 19.462 | 1.00 | 53.79 | C |
| ATOM | 2371 | CE1 | TYR | A | 308 | 46.426 | 42.426 | 21.643 | 1.00 | 54.22 | C |
| ATOM | 2372 | CE2 | TYR | A | 308 | 48.437 | 41.487 | 20.736 | 1.00 | 54.76 | C |
| ATOM | 2373 | CZ  | TYR | A | 308 | 47.670 | 41.857 | 21.824 | 1.00 | 55.10 | C |
| ATOM | 2374 | OH  | TYR | A | 308 | 48.146 | 41.659 | 23.101 | 1.00 | 56.68 | O |
| ATOM | 2375 | N   | PRO | A | 309 | 43.584 | 42.135 | 15.987 | 1.00 | 47.88 | N |
| ATOM | 2376 | CA  | PRO | A | 309 | 42.843 | 42.621 | 17.169 | 1.00 | 46.21 | C |
| ATOM | 2377 | C   | PRO | A | 309 | 42.139 | 41.503 | 17.952 | 1.00 | 43.75 | C |
| ATOM | 2378 | O   | PRO | A | 309 | 41.768 | 40.503 | 17.369 | 1.00 | 44.10 | O |
| ATOM | 2379 | CB  | PRO | A | 309 | 41.804 | 43.566 | 16.562 | 1.00 | 46.39 | C |
| ATOM | 2380 | CG  | PRO | A | 309 | 41.610 | 43.069 | 15.128 | 1.00 | 47.65 | C |
| ATOM | 2381 | CD  | PRO | A | 309 | 42.899 | 42.431 | 14.716 | 1.00 | 48.06 | C |
| ATOM | 2382 | N   | LEU | A | 310 | 41.973 | 41.672 | 19.256 | 1.00 | 40.94 | N |
| ATOM | 2383 | CA  | LEU | A | 310 | 41.349 | 40.650 | 20.093 | 1.00 | 38.75 | C |
| ATOM | 2384 | C   | LEU | A | 310 | 39.863 | 40.491 | 19.817 | 1.00 | 36.87 | C |
| ATOM | 2385 | O   | LEU | A | 310 | 39.148 | 41.474 | 19.610 | 1.00 | 37.02 | O |
| ATOM | 2386 | CB  | LEU | A | 310 | 41.499 | 41.017 | 21.566 | 1.00 | 38.63 | C |
| ATOM | 2387 | CG  | LEU | A | 310 | 42.571 | 40.351 | 22.435 | 1.00 | 37.97 | C |
| ATOM | 2388 | CD1 | LEU | A | 310 | 43.840 | 40.049 | 21.711 | 1.00 | 37.27 | C |
| ATOM | 2389 | CD2 | LEU | A | 310 | 42.836 | 41.234 | 23.637 | 1.00 | 37.27 | C |
| ATOM | 2390 | N   | LYS | A | 311 | 39.392 | 39.254 | 19.847 | 1.00 | 34.04 | N |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2391 | CA  | LYS | A | 311 | 37.972 | 38.998 | 19.702 | 1.00 | 32.20 | C |
| ATOM | 2392 | C   | LYS | A | 311 | 37.208 | 39.376 | 20.968 | 1.00 | 30.33 | C |
| ATOM | 2393 | O   | LYS | A | 311 | 37.760 | 39.421 | 22.072 | 1.00 | 29.17 | O |
| ATOM | 2394 | CB  | LYS | A | 311 | 37.733 | 37.564 | 19.371 | 1.00 | 32.59 | C |
| ATOM | 2395 | N   | ALA | A | 312 | 35.924 | 39.641 | 20.788 | 1.00 | 28.23 | N |
| ATOM | 2396 | CA  | ALA | A | 312 | 35.074 | 40.011 | 21.895 | 1.00 | 27.38 | C |
| ATOM | 2397 | C   | ALA | A | 312 | 35.148 | 38.973 | 23.005 | 1.00 | 26.28 | C |
| ATOM | 2398 | O   | ALA | A | 312 | 35.271 | 39.334 | 24.172 | 1.00 | 24.54 | O |
| ATOM | 2399 | CB  | ALA | A | 312 | 33.641 | 40.205 | 21.421 | 1.00 | 27.09 | C |
| ATOM | 2400 | N   | HIS | A | 313 | 35.101 | 37.689 | 22.649 | 1.00 | 25.72 | N |
| ATOM | 2401 | CA  | HIS | A | 313 | 35.086 | 36.669 | 23.674 | 1.00 | 25.82 | C |
| ATOM | 2402 | C   | HIS | A | 313 | 36.399 | 36.609 | 24.428 | 1.00 | 24.79 | C |
| ATOM | 2403 | O   | HIS | A | 313 | 36.428 | 36.183 | 25.557 | 1.00 | 24.19 | O |
| ATOM | 2404 | CB  | HIS | A | 313 | 34.688 | 35.293 | 23.129 | 1.00 | 26.92 | C |
| ATOM | 2405 | CG  | HIS | A | 313 | 35.741 | 34.641 | 22.303 | 1.00 | 29.84 | C |
| ATOM | 2406 | ND1 | HIS | A | 313 | 35.896 | 34.903 | 20.954 | 1.00 | 35.52 | N |
| ATOM | 2407 | CD2 | HIS | A | 313 | 36.702 | 33.746 | 22.627 | 1.00 | 33.54 | C |
| ATOM | 2408 | CE1 | HIS | A | 313 | 36.921 | 34.208 | 20.489 | 1.00 | 35.03 | C |
| ATOM | 2409 | NE2 | HIS | A | 313 | 37.424 | 33.491 | 21.481 | 1.00 | 35.78 | N |
| ATOM | 2410 | N   | GLN | A | 314 | 37.479 | 37.042 | 23.803 | 1.00 | 24.43 | N |
| ATOM | 2411 | CA  | GLN | A | 314 | 38.762 | 37.092 | 24.465 | 1.00 | 24.34 | C |
| ATOM | 2412 | C   | GLN | A | 314 | 38.762 | 38.226 | 25.510 | 1.00 | 24.39 | C |
| ATOM | 2413 | O   | GLN | A | 314 | 39.327 | 38.081 | 26.590 | 1.00 | 24.82 | O |
| ATOM | 2414 | CB  | GLN | A | 314 | 39.882 | 37.290 | 23.439 | 1.00 | 24.47 | C |
| ATOM | 2415 | CG  | GLN | A | 314 | 40.032 | 36.106 | 22.472 | 1.00 | 25.49 | C |
| ATOM | 2416 | CD  | GLN | A | 314 | 41.036 | 36.362 | 21.366 | 1.00 | 25.52 | C |
| ATOM | 2417 | OE1 | GLN | A | 314 | 40.878 | 37.287 | 20.563 | 1.00 | 27.59 | O |
| ATOM | 2418 | NE2 | GLN | A | 314 | 42.078 | 35.553 | 21.330 | 1.00 | 28.22 | N |
| ATOM | 2419 | N   | LYS | A | 315 | 38.113 | 39.337 | 25.196 | 1.00 | 23.51 | N |
| ATOM | 2420 | CA  | LYS | A | 315 | 38.000 | 40.423 | 26.154 | 1.00 | 23.79 | C |
| ATOM | 2421 | C   | LYS | A | 315 | 37.125 | 39.979 | 27.325 | 1.00 | 23.05 | C |
| ATOM | 2422 | O   | LYS | A | 315 | 37.373 | 40.347 | 28.465 | 1.00 | 21.38 | O |
| ATOM | 2423 | CB  | LYS | A | 315 | 37.421 | 41.667 | 25.504 | 1.00 | 24.09 | C |
| ATOM | 2424 | CG  | LYS | A | 315 | 38.382 | 42.286 | 24.533 | 1.00 | 26.96 | C |
| ATOM | 2425 | CD  | LYS | A | 315 | 37.849 | 43.552 | 23.947 | 1.00 | 31.28 | C |
| ATOM | 2426 | CE  | LYS | A | 315 | 38.856 | 44.156 | 22.977 | 1.00 | 34.34 | C |
| ATOM | 2427 | NZ  | LYS | A | 315 | 38.207 | 45.098 | 22.005 | 1.00 | 36.25 | N |
| ATOM | 2428 | N   | VAL | A | 316 | 36.109 | 39.177 | 27.041 | 1.00 | 22.30 | N |
| ATOM | 2429 | CA  | VAL | A | 316 | 35.276 | 38.673 | 28.113 | 1.00 | 22.39 | C |
| ATOM | 2430 | C   | VAL | A | 316 | 36.124 | 37.800 | 29.063 | 1.00 | 22.29 | C |
| ATOM | 2431 | O   | VAL | A | 316 | 36.040 | 37.932 | 30.274 | 1.00 | 21.27 | O |
| ATOM | 2432 | CB  | VAL | A | 316 | 34.065 | 37.887 | 27.595 | 1.00 | 22.03 | C |
| ATOM | 2433 | CG1 | VAL | A | 316 | 33.309 | 37.282 | 28.750 | 1.00 | 21.64 | C |
| ATOM | 2434 | CG2 | VAL | A | 316 | 33.123 | 38.796 | 26.802 | 1.00 | 22.46 | C |
| ATOM | 2435 | N   | ALA | A | 317 | 36.964 | 36.941 | 28.499 | 1.00 | 22.09 | N |
| ATOM | 2436 | CA  | ALA | A | 317 | 37.848 | 36.086 | 29.295 | 1.00 | 21.98 | C |
| ATOM | 2437 | C   | ALA | A | 317 | 38.783 | 36.916 | 30.164 | 1.00 | 21.61 | C |
| ATOM | 2438 | O   | ALA | A | 317 | 39.042 | 36.573 | 31.300 | 1.00 | 21.05 | O |
| ATOM | 2439 | CB  | ALA | A | 317 | 38.668 | 35.147 | 28.380 | 1.00 | 22.01 | C |
| ATOM | 2440 | N   | ILE | A | 318 | 39.273 | 38.016 | 29.606 | 1.00 | 21.45 | N |
| ATOM | 2441 | CA  | ILE | A | 318 | 40.162 | 38.917 | 30.318 | 1.00 | 21.24 | C |
| ATOM | 2442 | C   | ILE | A | 318 | 39.431 | 39.511 | 31.524 | 1.00 | 21.38 | C |
| ATOM | 2443 | O   | ILE | A | 318 | 39.937 | 39.462 | 32.646 | 1.00 | 20.76 | O |
| ATOM | 2444 | CB  | ILE | A | 318 | 40.709 | 40.023 | 29.377 | 1.00 | 20.58 | C |
| ATOM | 2445 | CG1 | ILE | A | 318 | 41.715 | 39.434 | 28.400 | 1.00 | 21.19 | C |
| ATOM | 2446 | CG2 | ILE | A | 318 | 41.354 | 41.167 | 30.185 | 1.00 | 20.20 | C |
| ATOM | 2447 | CD1 | ILE | A | 318 | 42.223 | 40.419 | 27.353 | 1.00 | 21.35 | C |
| ATOM | 2448 | N   | MET | A | 319 | 38.234 | 40.030 | 31.287 | 1.00 | 20.83 | N |
| ATOM | 2449 | CA  | MET | A | 319 | 37.446 | 40.622 | 32.355 | 1.00 | 21.31 | C |
| ATOM | 2450 | C   | MET | A | 319 | 37.154 | 39.617 | 33.454 | 1.00 | 21.52 | C |
| ATOM | 2451 | O   | MET | A | 319 | 37.326 | 39.911 | 34.651 | 1.00 | 21.13 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2452 | CB  | MET | A | 319 | 36.177 | 41.260 | 31.818 | 1.00 | 21.01 | C |
| ATOM | 2453 | CG  | MET | A | 319 | 36.423 | 42.519 | 30.971 | 1.00 | 21.17 | C |
| ATOM | 2454 | SD  | MET | A | 319 | 34.860 | 43.346 | 30.459 | 1.00 | 22.71 | S |
| ATOM | 2455 | CE  | MET | A | 319 | 34.204 | 42.152 | 29.206 | 1.00 | 22.13 | C |
| ATOM | 2456 | N   | ARG | A | 320 | 36.767 | 38.408 | 33.068 | 1.00 | 21.34 | N |
| ATOM | 2457 | CA  | ARG | A | 320 | 36.532 | 37.399 | 34.075 | 1.00 | 21.12 | C |
| ATOM | 2458 | C   | ARG | A | 320 | 37.801 | 37.186 | 34.898 | 1.00 | 21.25 | C |
| ATOM | 2459 | O   | ARG | A | 320 | 37.747 | 37.064 | 36.122 | 1.00 | 21.48 | O |
| ATOM | 2460 | CB  | ARG | A | 320 | 36.102 | 36.095 | 33.427 | 1.00 | 21.01 | C |
| ATOM | 2461 | CG  | ARG | A | 320 | 34.723 | 36.145 | 32.741 | 1.00 | 20.63 | C |
| ATOM | 2462 | CD  | ARG | A | 320 | 34.324 | 34.795 | 32.142 | 1.00 | 18.73 | C |
| ATOM | 2463 | NE  | ARG | A | 320 | 34.225 | 33.824 | 33.225 | 1.00 | 19.25 | N |
| ATOM | 2464 | CZ  | ARG | A | 320 | 33.247 | 33.809 | 34.115 | 1.00 | 19.86 | C |
| ATOM | 2465 | NH1 | ARG | A | 320 | 32.259 | 34.689 | 34.062 | 1.00 | 21.08 | N |
| ATOM | 2466 | NH2 | ARG | A | 320 | 33.263 | 32.923 | 35.081 | 1.00 | 23.29 | N |
| ATOM | 2467 | N   | ASN | A | 321 | 38.947 | 37.123 | 34.231 | 1.00 | 20.94 | N |
| ATOM | 2468 | CA  | ASN | A | 321 | 40.184 | 36.855 | 34.939 | 1.00 | 20.88 | C |
| ATOM | 2469 | C   | ASN | A | 321 | 40.535 | 37.981 | 35.916 | 1.00 | 20.93 | C |
| ATOM | 2470 | O   | ASN | A | 321 | 40.962 | 37.716 | 37.047 | 1.00 | 21.77 | O |
| ATOM | 2471 | CB  | ASN | A | 321 | 41.324 | 36.552 | 33.958 | 1.00 | 21.04 | C |
| ATOM | 2472 | CG  | ASN | A | 321 | 41.288 | 35.099 | 33.447 | 1.00 | 22.80 | C |
| ATOM | 2473 | OD1 | ASN | A | 321 | 40.924 | 34.193 | 34.185 | 1.00 | 23.97 | O |
| ATOM | 2474 | ND2 | ASN | A | 321 | 41.666 | 34.887 | 32.193 | 1.00 | 21.35 | N |
| ATOM | 2475 | N   | ILE | A | 322 | 40.355 | 39.233 | 35.505 | 1.00 | 20.14 | N |
| ATOM | 2476 | CA  | ILE | A | 322 | 40.633 | 40.336 | 36.408 | 1.00 | 20.06 | C |
| ATOM | 2477 | C   | ILE | A | 322 | 39.742 | 40.196 | 37.650 | 1.00 | 19.42 | C |
| ATOM | 2478 | O   | ILE | A | 322 | 40.207 | 40.345 | 38.767 | 1.00 | 18.73 | O |
| ATOM | 2479 | CB  | ILE | A | 322 | 40.372 | 41.690 | 35.715 | 1.00 | 20.21 | C |
| ATOM | 2480 | CG1 | ILE | A | 322 | 41.320 | 41.894 | 34.535 | 1.00 | 21.54 | C |
| ATOM | 2481 | CG2 | ILE | A | 322 | 40.504 | 42.823 | 36.699 | 1.00 | 20.53 | C |
| ATOM | 2482 | CD1 | ILE | A | 322 | 42.806 | 41.798 | 34.868 | 1.00 | 24.56 | C |
| ATOM | 2483 | N   | GLU | A | 323 | 38.458 | 39.904 | 37.454 | 1.00 | 18.94 | N |
| ATOM | 2484 | CA  | GLU | A | 323 | 37.553 | 39.757 | 38.576 | 1.00 | 18.98 | C |
| ATOM | 2485 | C   | GLU | A | 323 | 38.027 | 38.651 | 39.492 | 1.00 | 19.33 | C |
| ATOM | 2486 | O   | GLU | A | 323 | 38.084 | 38.832 | 40.707 | 1.00 | 19.05 | O |
| ATOM | 2487 | CB  | GLU | A | 323 | 36.113 | 39.538 | 38.106 | 1.00 | 19.25 | C |
| ATOM | 2488 | CG  | GLU | A | 323 | 35.518 | 40.803 | 37.484 | 1.00 | 19.34 | C |
| ATOM | 2489 | CD  | GLU | A | 323 | 34.143 | 40.616 | 36.855 | 1.00 | 18.71 | C |
| ATOM | 2490 | OE1 | GLU | A | 323 | 33.183 | 40.332 | 37.573 | 1.00 | 19.19 | O |
| ATOM | 2491 | OE2 | GLU | A | 323 | 34.024 | 40.805 | 35.636 | 1.00 | 19.56 | O |
| ATOM | 2492 | N   | LYS | A | 324 | 38.425 | 37.528 | 38.908 | 1.00 | 19.55 | N |
| ATOM | 2493 | CA  | LYS | A | 324 | 38.874 | 36.379 | 39.693 | 1.00 | 20.24 | C |
| ATOM | 2494 | C   | LYS | A | 324 | 40.115 | 36.707 | 40.513 | 1.00 | 20.68 | C |
| ATOM | 2495 | O   | LYS | A | 324 | 40.157 | 36.405 | 41.699 | 1.00 | 20.83 | O |
| ATOM | 2496 | CB  | LYS | A | 324 | 39.175 | 35.175 | 38.789 | 1.00 | 20.07 | C |
| ATOM | 2497 | CG  | LYS | A | 324 | 37.924 | 34.507 | 38.212 | 1.00 | 20.57 | C |
| ATOM | 2498 | CD  | LYS | A | 324 | 38.331 | 33.318 | 37.350 | 1.00 | 20.28 | C |
| ATOM | 2499 | CE  | LYS | A | 324 | 37.137 | 32.689 | 36.621 | 1.00 | 19.29 | C |
| ATOM | 2500 | NZ  | LYS | A | 324 | 37.596 | 31.460 | 35.876 | 1.00 | 17.17 | N |
| ATOM | 2501 | N   | MET | A | 325 | 41.112 | 37.320 | 39.885 | 1.00 | 21.21 | N |
| ATOM | 2502 | CA  | MET | A | 325 | 42.366 | 37.657 | 40.568 | 1.00 | 22.87 | C |
| ATOM | 2503 | C   | MET | A | 325 | 42.162 | 38.665 | 41.699 | 1.00 | 22.44 | C |
| ATOM | 2504 | O   | MET | A | 325 | 42.763 | 38.560 | 42.771 | 1.00 | 22.08 | O |
| ATOM | 2505 | CB  | MET | A | 325 | 43.380 | 38.232 | 39.572 | 1.00 | 23.32 | C |
| ATOM | 2506 | CG  | MET | A | 325 | 43.993 | 37.195 | 38.671 | 1.00 | 27.47 | C |
| ATOM | 2507 | SD  | MET | A | 325 | 44.795 | 37.924 | 37.197 | 1.00 | 35.56 | S |
| ATOM | 2508 | CE  | MET | A | 325 | 45.664 | 39.189 | 38.009 | 1.00 | 34.71 | C |
| ATOM | 2509 | N   | LEU | A | 326 | 41.309 | 39.641 | 41.452 | 1.00 | 22.71 | N |
| ATOM | 2510 | CA  | LEU | A | 326 | 41.043 | 40.670 | 42.449 | 1.00 | 23.24 | C |
| ATOM | 2511 | C   | LEU | A | 326 | 40.385 | 40.073 | 43.679 | 1.00 | 23.15 | C |
| ATOM | 2512 | O   | LEU | A | 326 | 40.735 | 40.417 | 44.795 | 1.00 | 22.40 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2513 | CB  | LEU | A | 326 | 40.151 | 41.735 | 41.865 | 1.00 | 23.01 | C |
| ATOM | 2514 | CG  | LEU | A | 326 | 40.677 | 43.139 | 41.625 | 1.00 | 25.86 | C |
| ATOM | 2515 | CD1 | LEU | A | 326 | 42.187 | 43.277 | 41.529 | 1.00 | 26.53 | C |
| ATOM | 2516 | CD2 | LEU | A | 326 | 39.986 | 43.672 | 40.377 | 1.00 | 25.54 | C |
| ATOM | 2517 | N   | GLY | A | 327 | 39.441 | 39.164 | 43.460 | 1.00 | 23.29 | N |
| ATOM | 2518 | CA  | GLY | A | 327 | 38.760 | 38.489 | 44.547 | 1.00 | 23.97 | C |
| ATOM | 2519 | C   | GLY | A | 327 | 39.728 | 37.723 | 45.418 | 1.00 | 24.63 | C |
| ATOM | 2520 | O   | GLY | A | 327 | 39.659 | 37.783 | 46.649 | 1.00 | 24.75 | O |
| ATOM | 2521 | N   | GLU | A | 328 | 40.644 | 37.002 | 44.778 | 1.00 | 25.03 | N |
| ATOM | 2522 | CA  | GLU | A | 328 | 41.671 | 36.265 | 45.506 | 1.00 | 26.08 | C |
| ATOM | 2523 | C   | GLU | A | 328 | 42.661 | 37.180 | 46.223 | 1.00 | 25.43 | C |
| ATOM | 2524 | O   | GLU | A | 328 | 43.029 | 36.926 | 47.367 | 1.00 | 25.16 | O |
| ATOM | 2525 | CB  | GLU | A | 328 | 42.442 | 35.368 | 44.546 | 1.00 | 26.76 | C |
| ATOM | 2526 | CG  | GLU | A | 328 | 41.576 | 34.278 | 43.947 | 1.00 | 30.36 | C |
| ATOM | 2527 | CD  | GLU | A | 328 | 41.719 | 32.957 | 44.676 | 1.00 | 35.76 | C |
| ATOM | 2528 | OE1 | GLU | A | 328 | 42.091 | 32.986 | 45.878 | 1.00 | 38.79 | O |
| ATOM | 2529 | OE2 | GLU | A | 328 | 41.483 | 31.896 | 44.034 | 1.00 | 38.82 | O |
| ATOM | 2530 | N   | ALA | A | 329 | 43.094 | 38.240 | 45.552 | 1.00 | 24.91 | N |
| ATOM | 2531 | CA  | ALA | A | 329 | 44.102 | 39.119 | 46.134 | 1.00 | 24.95 | C |
| ATOM | 2532 | C   | ALA | A | 329 | 43.535 | 39.929 | 47.285 | 1.00 | 24.94 | C |
| ATOM | 2533 | O   | ALA | A | 329 | 44.197 | 40.147 | 48.276 | 1.00 | 24.57 | O |
| ATOM | 2534 | CB  | ALA | A | 329 | 44.682 | 40.022 | 45.088 | 1.00 | 24.88 | C |
| ATOM | 2535 | N   | LEU | A | 330 | 42.290 | 40.354 | 47.161 | 1.00 | 25.47 | N |
| ATOM | 2536 | CA  | LEU | A | 330 | 41.672 | 41.133 | 48.219 | 1.00 | 26.16 | C |
| ATOM | 2537 | C   | LEU | A | 330 | 41.212 | 40.265 | 49.379 | 1.00 | 26.80 | C |
| ATOM | 2538 | O   | LEU | A | 330 | 40.994 | 40.761 | 50.471 | 1.00 | 27.00 | O |
| ATOM | 2539 | CB  | LEU | A | 330 | 40.504 | 41.930 | 47.669 | 1.00 | 26.08 | C |
| ATOM | 2540 | CG  | LEU | A | 330 | 40.954 | 42.981 | 46.653 | 1.00 | 26.04 | C |
| ATOM | 2541 | CD1 | LEU | A | 330 | 39.760 | 43.489 | 45.888 | 1.00 | 26.16 | C |
| ATOM | 2542 | CD2 | LEU | A | 330 | 41.688 | 44.134 | 47.353 | 1.00 | 26.65 | C |
| ATOM | 2543 | N   | GLY | A | 331 | 41.037 | 38.977 | 49.126 | 1.00 | 27.87 | N |
| ATOM | 2544 | CA  | GLY | A | 331 | 40.645 | 38.039 | 50.158 | 1.00 | 28.89 | C |
| ATOM | 2545 | C   | GLY | A | 331 | 39.176 | 38.086 | 50.526 | 1.00 | 29.43 | C |
| ATOM | 2546 | O   | GLY | A | 331 | 38.763 | 37.435 | 51.478 | 1.00 | 30.62 | O |
| ATOM | 2547 | N   | ASN | A | 332 | 38.400 | 38.887 | 49.808 | 1.00 | 29.59 | N |
| ATOM | 2548 | CA  | ASN | A | 332 | 36.963 | 38.995 | 50.023 | 1.00 | 29.64 | C |
| ATOM | 2549 | C   | ASN | A | 332 | 36.367 | 39.500 | 48.718 | 1.00 | 29.00 | C |
| ATOM | 2550 | O   | ASN | A | 332 | 36.649 | 40.605 | 48.303 | 1.00 | 28.70 | O |
| ATOM | 2551 | CB  | ASN | A | 332 | 36.656 | 39.973 | 51.156 | 1.00 | 30.15 | C |
| ATOM | 2552 | CG  | ASN | A | 332 | 35.162 | 40.094 | 51.441 | 1.00 | 31.82 | C |
| ATOM | 2553 | OD1 | ASN | A | 332 | 34.335 | 39.531 | 50.734 | 1.00 | 34.71 | O |
| ATOM | 2554 | ND2 | ASN | A | 332 | 34.818 | 40.818 | 52.504 | 1.00 | 35.11 | N |
| ATOM | 2555 | N   | PRO | A | 333 | 35.528 | 38.706 | 48.081 | 1.00 | 28.53 | N |
| ATOM | 2556 | CA  | PRO | A | 333 | 35.001 | 39.075 | 46.771 | 1.00 | 28.25 | C |
| ATOM | 2557 | C   | PRO | A | 333 | 34.176 | 40.343 | 46.807 | 1.00 | 27.91 | C |
| ATOM | 2558 | O   | PRO | A | 333 | 34.033 | 40.984 | 45.776 | 1.00 | 26.99 | O |
| ATOM | 2559 | CB  | PRO | A | 333 | 34.120 | 37.893 | 46.368 | 1.00 | 28.16 | C |
| ATOM | 2560 | CG  | PRO | A | 333 | 34.137 | 36.938 | 47.468 | 1.00 | 28.91 | C |
| ATOM | 2561 | CD  | PRO | A | 333 | 35.022 | 37.415 | 48.561 | 1.00 | 28.96 | C |
| ATOM | 2562 | N   | GLN | A | 334 | 33.638 | 40.701 | 47.965 | 1.00 | 27.80 | N |
| ATOM | 2563 | CA  | GLN | A | 334 | 32.814 | 41.896 | 48.039 | 1.00 | 27.97 | C |
| ATOM | 2564 | C   | GLN | A | 334 | 33.665 | 43.155 | 47.975 | 1.00 | 26.77 | C |
| ATOM | 2565 | O   | GLN | A | 334 | 33.144 | 44.245 | 47.764 | 1.00 | 26.51 | O |
| ATOM | 2566 | CB  | GLN | A | 334 | 31.906 | 41.867 | 49.278 | 1.00 | 28.98 | C |
| ATOM | 2567 | CG  | GLN | A | 334 | 30.675 | 40.969 | 49.038 | 1.00 | 32.17 | C |
| ATOM | 2568 | CD  | GLN | A | 334 | 29.661 | 40.962 | 50.175 | 1.00 | 35.54 | C |
| ATOM | 2569 | OE1 | GLN | A | 334 | 29.682 | 41.840 | 51.048 | 1.00 | 37.92 | O |
| ATOM | 2570 | NE2 | GLN | A | 334 | 28.760 | 39.961 | 50.163 | 1.00 | 36.72 | N |
| ATOM | 2571 | N   | GLU | A | 335 | 34.974 | 43.007 | 48.132 | 1.00 | 25.19 | N |
| ATOM | 2572 | CA  | GLU | A | 335 | 35.860 | 44.151 | 48.018 | 1.00 | 24.41 | C |
| ATOM | 2573 | C   | GLU | A | 335 | 36.170 | 44.466 | 46.537 | 1.00 | 22.68 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2574 | O   | GLU | A | 335 | 36.700 | 45.521 | 46.228 | 1.00 | 21.42 | O |
| ATOM | 2575 | CB  | GLU | A | 335 | 37.150 | 43.928 | 48.835 | 1.00 | 24.98 | C |
| ATOM | 2576 | CG  | GLU | A | 335 | 36.974 | 44.148 | 50.343 | 1.00 | 27.94 | C |
| ATOM | 2577 | CD  | GLU | A | 335 | 38.264 | 44.055 | 51.139 | 1.00 | 31.85 | C |
| ATOM | 2578 | OE1 | GLU | A | 335 | 39.248 | 44.736 | 50.777 | 1.00 | 34.79 | O |
| ATOM | 2579 | OE2 | GLU | A | 335 | 38.298 | 43.312 | 52.158 | 1.00 | 36.87 | O |
| ATOM | 2580 | N   | VAL | A | 336 | 35.809 | 43.566 | 45.625 | 1.00 | 21.32 | N |
| ATOM | 2581 | CA  | VAL | A | 336 | 36.113 | 43.751 | 44.201 | 1.00 | 20.37 | C |
| ATOM | 2582 | C   | VAL | A | 336 | 35.541 | 45.034 | 43.603 | 1.00 | 20.01 | C |
| ATOM | 2583 | O   | VAL | A | 336 | 36.247 | 45.798 | 42.954 | 1.00 | 19.07 | O |
| ATOM | 2584 | CB  | VAL | A | 336 | 35.647 | 42.554 | 43.371 | 1.00 | 20.60 | C |
| ATOM | 2585 | CG1 | VAL | A | 336 | 35.785 | 42.841 | 41.883 | 1.00 | 21.06 | C |
| ATOM | 2586 | CG2 | VAL | A | 336 | 36.463 | 41.316 | 43.743 | 1.00 | 20.68 | C |
| ATOM | 2587 | N   | GLY | A | 337 | 34.260 | 45.275 | 43.842 | 1.00 | 19.61 | N |
| ATOM | 2588 | CA  | GLY | A | 337 | 33.593 | 46.437 | 43.317 | 1.00 | 19.45 | C |
| ATOM | 2589 | C   | GLY | A | 337 | 34.205 | 47.760 | 43.731 | 1.00 | 19.51 | C |
| ATOM | 2590 | O   | GLY | A | 337 | 34.522 | 48.576 | 42.871 | 1.00 | 18.93 | O |
| ATOM | 2591 | N   | PRO | A | 338 | 34.333 | 48.010 | 45.032 | 1.00 | 20.41 | N |
| ATOM | 2592 | CA  | PRO | A | 338 | 34.959 | 49.253 | 45.503 | 1.00 | 20.40 | C |
| ATOM | 2593 | C   | PRO | A | 338 | 36.368 | 49.500 | 44.923 | 1.00 | 20.13 | C |
| ATOM | 2594 | O   | PRO | A | 338 | 36.674 | 50.630 | 44.548 | 1.00 | 19.20 | O |
| ATOM | 2595 | CB  | PRO | A | 338 | 34.960 | 49.092 | 47.035 | 1.00 | 20.63 | C |
| ATOM | 2596 | CG  | PRO | A | 338 | 33.749 | 48.261 | 47.298 | 1.00 | 21.17 | C |
| ATOM | 2597 | CD  | PRO | A | 338 | 33.782 | 47.221 | 46.151 | 1.00 | 20.95 | C |
| ATOM | 2598 | N   | LEU | A | 339 | 37.199 | 48.470 | 44.831 | 1.00 | 20.34 | N |
| ATOM | 2599 | CA  | LEU | A | 339 | 38.518 | 48.655 | 44.234 | 1.00 | 20.55 | C |
| ATOM | 2600 | C   | LEU | A | 339 | 38.382 | 49.060 | 42.768 | 1.00 | 20.06 | C |
| ATOM | 2601 | O   | LEU | A | 339 | 39.020 | 50.019 | 42.330 | 1.00 | 19.61 | O |
| ATOM | 2602 | CB  | LEU | A | 339 | 39.383 | 47.408 | 44.358 | 1.00 | 20.81 | C |
| ATOM | 2603 | CG  | LEU | A | 339 | 40.855 | 47.618 | 43.943 | 1.00 | 22.54 | C |
| ATOM | 2604 | CD1 | LEU | A | 339 | 41.809 | 46.817 | 44.786 | 1.00 | 25.30 | C |
| ATOM | 2605 | CD2 | LEU | A | 339 | 41.035 | 47.209 | 42.496 | 1.00 | 23.17 | C |
| ATOM | 2606 | N   | LEU | A | 340 | 37.526 | 48.361 | 42.023 | 1.00 | 19.51 | N |
| ATOM | 2607 | CA  | LEU | A | 340 | 37.327 | 48.687 | 40.600 | 1.00 | 19.36 | C |
| ATOM | 2608 | C   | LEU | A | 340 | 36.827 | 50.120 | 40.427 | 1.00 | 19.30 | C |
| ATOM | 2609 | O   | LEU | A | 340 | 37.318 | 50.861 | 39.566 | 1.00 | 17.55 | O |
| ATOM | 2610 | CB  | LEU | A | 340 | 36.361 | 47.721 | 39.952 | 1.00 | 19.31 | C |
| ATOM | 2611 | CG  | LEU | A | 340 | 36.929 | 46.333 | 39.637 | 1.00 | 21.99 | C |
| ATOM | 2612 | CD1 | LEU | A | 340 | 35.842 | 45.506 | 39.069 | 1.00 | 22.03 | C |
| ATOM | 2613 | CD2 | LEU | A | 340 | 38.140 | 46.390 | 38.673 | 1.00 | 21.20 | C |
| ATOM | 2614 | N   | ASN | A | 341 | 35.879 | 50.521 | 41.270 | 1.00 | 19.17 | N |
| ATOM | 2615 | CA  | ASN | A | 341 | 35.369 | 51.887 | 41.232 | 1.00 | 20.20 | C |
| ATOM | 2616 | C   | ASN | A | 341 | 36.465 | 52.914 | 41.530 | 1.00 | 19.98 | C |
| ATOM | 2617 | O   | ASN | A | 341 | 36.598 | 53.920 | 40.848 | 1.00 | 19.61 | O |
| ATOM | 2618 | CB  | ASN | A | 341 | 34.181 | 52.043 | 42.196 | 1.00 | 20.66 | C |
| ATOM | 2619 | CG  | ASN | A | 341 | 32.898 | 51.459 | 41.619 | 1.00 | 24.17 | C |
| ATOM | 2620 | OD1 | ASN | A | 341 | 32.484 | 51.843 | 40.531 | 1.00 | 30.93 | O |
| ATOM | 2621 | ND2 | ASN | A | 341 | 32.294 | 50.499 | 42.317 | 1.00 | 26.37 | N |
| ATOM | 2622 | N   | THR | A | 342 | 37.245 | 52.633 | 42.558 | 1.00 | 20.07 | N |
| ATOM | 2623 | CA  | THR | A | 342 | 38.351 | 53.489 | 42.939 | 1.00 | 20.49 | C |
| ATOM | 2624 | C   | THR | A | 342 | 39.322 | 53.613 | 41.763 | 1.00 | 20.27 | C |
| ATOM | 2625 | O   | THR | A | 342 | 39.835 | 54.688 | 41.502 | 1.00 | 19.66 | O |
| ATOM | 2626 | CB  | THR | A | 342 | 39.001 | 52.909 | 44.189 | 1.00 | 20.82 | C |
| ATOM | 2627 | OG1 | THR | A | 342 | 38.123 | 53.124 | 45.320 | 1.00 | 22.13 | O |
| ATOM | 2628 | CG2 | THR | A | 342 | 40.308 | 53.625 | 44.545 | 1.00 | 21.01 | C |
| ATOM | 2629 | N   | MET | A | 343 | 39.517 | 52.525 | 41.024 | 1.00 | 20.30 | N |
| ATOM | 2630 | CA  | MET | A | 343 | 40.402 | 52.543 | 39.873 | 1.00 | 20.66 | C |
| ATOM | 2631 | C   | MET | A | 343 | 39.932 | 53.445 | 38.758 | 1.00 | 20.29 | C |
| ATOM | 2632 | O   | MET | A | 343 | 40.750 | 54.119 | 38.129 | 1.00 | 19.31 | O |
| ATOM | 2633 | CB  | MET | A | 343 | 40.560 | 51.157 | 39.270 | 1.00 | 20.76 | C |
| ATOM | 2634 | CG  | MET | A | 343 | 41.810 | 50.453 | 39.625 | 1.00 | 23.39 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2635 | SD  | MET | A | 343 | 42.247 | 49.059 | 38.524 | 1.00 | 25.69 | S |
| ATOM | 2636 | CE  | MET | A | 343 | 41.161 | 48.058 | 38.968 | 1.00 | 26.74 | C |
| ATOM | 2637 | N   | ILE | A | 344 | 38.631 | 53.438 | 38.466 | 1.00 | 20.76 | N |
| ATOM | 2638 | CA  | ILE | A | 344 | 38.167 | 54.187 | 37.312 | 1.00 | 21.23 | C |
| ATOM | 2639 | C   | ILE | A | 344 | 37.648 | 55.577 | 37.565 | 1.00 | 20.71 | C |
| ATOM | 2640 | O   | ILE | A | 344 | 37.763 | 56.403 | 36.666 | 1.00 | 20.65 | O |
| ATOM | 2641 | CB  | ILE | A | 344 | 37.109 | 53.400 | 36.458 | 1.00 | 22.07 | C |
| ATOM | 2642 | CG1 | ILE | A | 344 | 35.710 | 53.613 | 36.992 | 1.00 | 23.91 | C |
| ATOM | 2643 | CG2 | ILE | A | 344 | 37.482 | 51.943 | 36.352 | 1.00 | 24.35 | C |
| ATOM | 2644 | CD1 | ILE | A | 344 | 34.650 | 53.199 | 36.033 | 1.00 | 28.26 | C |
| ATOM | 2645 | N   | LYS | A | 345 | 37.069 | 55.886 | 38.726 | 1.00 | 20.84 | N |
| ATOM | 2646 | CA  | LYS | A | 345 | 36.482 | 57.231 | 38.817 | 1.00 | 21.15 | C |
| ATOM | 2647 | C   | LYS | A | 345 | 37.464 | 58.376 | 38.784 | 1.00 | 19.86 | C |
| ATOM | 2648 | O   | LYS | A | 345 | 38.459 | 58.429 | 39.517 | 1.00 | 19.23 | O |
| ATOM | 2649 | CB  | LYS | A | 345 | 35.438 | 57.451 | 39.922 | 1.00 | 22.66 | C |
| ATOM | 2650 | CG  | LYS | A | 345 | 35.562 | 56.714 | 41.190 | 1.00 | 27.82 | C |
| ATOM | 2651 | CD  | LYS | A | 345 | 34.214 | 56.021 | 41.489 | 1.00 | 30.51 | C |
| ATOM | 2652 | CE  | LYS | A | 345 | 33.398 | 56.782 | 42.502 | 1.00 | 32.51 | C |
| ATOM | 2653 | NZ  | LYS | A | 345 | 34.069 | 56.806 | 43.829 | 1.00 | 37.63 | N |
| ATOM | 2654 | N   | GLY | A | 346 | 37.143 | 59.307 | 37.899 | 1.00 | 18.18 | N |
| ATOM | 2655 | CA  | GLY | A | 346 | 37.978 | 60.453 | 37.644 | 1.00 | 17.22 | C |
| ATOM | 2656 | C   | GLY | A | 346 | 39.303 | 60.105 | 36.978 | 1.00 | 16.31 | C |
| ATOM | 2657 | O   | GLY | A | 346 | 40.172 | 60.949 | 36.889 | 1.00 | 16.63 | O |
| ATOM | 2658 | N   | ARG | A | 347 | 39.453 | 58.872 | 36.531 | 1.00 | 16.85 | N |
| ATOM | 2659 | CA  | ARG | A | 347 | 40.697 | 58.413 | 35.904 | 1.00 | 17.52 | C |
| ATOM | 2660 | C   | ARG | A | 347 | 40.469 | 57.811 | 34.502 | 1.00 | 17.57 | C |
| ATOM | 2661 | O   | ARG | A | 347 | 41.178 | 58.143 | 33.559 | 1.00 | 17.10 | O |
| ATOM | 2662 | CB  | ARG | A | 347 | 41.379 | 57.384 | 36.812 | 1.00 | 17.20 | C |
| ATOM | 2663 | CG  | ARG | A | 347 | 41.822 | 57.949 | 38.181 | 1.00 | 16.77 | C |
| ATOM | 2664 | CD  | ARG | A | 347 | 43.287 | 57.491 | 38.583 | 1.00 | 18.88 | C |
| ATOM | 2665 | NE  | ARG | A | 347 | 43.254 | 56.087 | 38.618 | 1.00 | 17.77 | N |
| ATOM | 2666 | CZ  | ARG | A | 347 | 44.115 | 55.220 | 38.149 | 1.00 | 16.11 | C |
| ATOM | 2667 | NH1 | ARG | A | 347 | 45.323 | 55.512 | 37.658 | 1.00 | 16.59 | N |
| ATOM | 2668 | NH2 | ARG | A | 347 | 43.734 | 53.978 | 38.276 | 1.00 | 13.22 | N |
| ATOM | 2669 | N   | TYR | A | 348 | 39.472 | 56.954 | 34.375 | 1.00 | 18.74 | N |
| ATOM | 2670 | CA  | TYR | A | 348 | 39.138 | 56.317 | 33.091 | 1.00 | 20.48 | C |
| ATOM | 2671 | C   | TYR | A | 348 | 37.674 | 56.499 | 32.671 | 1.00 | 21.75 | C |
| ATOM | 2672 | O   | TYR | A | 348 | 37.296 | 56.047 | 31.596 | 1.00 | 22.39 | O |
| ATOM | 2673 | CB  | TYR | A | 348 | 39.411 | 54.800 | 33.124 | 1.00 | 19.97 | C |
| ATOM | 2674 | CG  | TYR | A | 348 | 40.874 | 54.384 | 33.199 | 1.00 | 19.65 | C |
| ATOM | 2675 | CD1 | TYR | A | 348 | 41.661 | 54.310 | 32.054 | 1.00 | 18.48 | C |
| ATOM | 2676 | CD2 | TYR | A | 348 | 41.458 | 54.051 | 34.414 | 1.00 | 17.73 | C |
| ATOM | 2677 | CE1 | TYR | A | 348 | 42.986 | 53.921 | 32.122 | 1.00 | 19.00 | C |
| ATOM | 2678 | CE2 | TYR | A | 348 | 42.775 | 53.667 | 34.494 | 1.00 | 18.72 | C |
| ATOM | 2679 | CZ  | TYR | A | 348 | 43.543 | 53.600 | 33.339 | 1.00 | 18.96 | C |
| ATOM | 2680 | OH  | TYR | A | 348 | 44.856 | 53.203 | 33.419 | 1.00 | 17.77 | O |
| ATOM | 2681 | N   | ASN | A | 349 | 36.837 | 57.123 | 33.488 | 1.00 | 23.99 | N |
| ATOM | 2682 | CA  | ASN | A | 349 | 35.429 | 57.244 | 33.089 | 1.00 | 26.57 | C |
| ATOM | 2683 | C   | ASN | A | 349 | 34.947 | 58.611 | 32.689 | 1.00 | 27.62 | C |
| ATOM | 2684 | O   | ASN | A | 349 | 35.646 | 59.606 | 32.655 | 1.00 | 28.49 | O |
| ATOM | 2685 | CB  | ASN | A | 349 | 34.496 | 56.720 | 34.150 | 1.00 | 26.11 | C |
| ATOM | 2686 | CG  | ASN | A | 349 | 34.511 | 57.552 | 35.386 | 1.00 | 28.01 | C |
| ATOM | 2687 | OD1 | ASN | A | 349 | 35.282 | 58.518 | 35.517 | 1.00 | 29.49 | O |
| ATOM | 2688 | ND2 | ASN | A | 349 | 33.658 | 57.173 | 36.342 | 1.00 | 31.84 | N |
| ATOM | 2689 | OXT | ASN | A | 349 | 33.761 | 58.686 | 32.399 | 1.00 | 31.04 | O |
| TER  | 2690 |     | ASN | A | 349 |        |        |        |      |       |   |
| ATOM | 2691 | N   | LEU | S | 795 | 45.837 | 35.555 | 30.600 | 1.00 | 35.49 | N |
| ATOM | 2692 | CA  | LEU | S | 795 | 44.757 | 36.539 | 30.946 | 1.00 | 35.77 | C |
| ATOM | 2693 | C   | LEU | S | 795 | 43.580 | 36.250 | 30.030 | 1.00 | 35.54 | C |
| ATOM | 2694 | O   | LEU | S | 795 | 42.418 | 36.338 | 30.412 | 1.00 | 34.79 | O |
| ATOM | 2695 | CB  | LEU | S | 795 | 45.257 | 37.967 | 30.787 | 1.00 | 36.01 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2696 | CG  | LEU | S | 795 | 44.695 | 38.978 | 31.791 | 1.00 | 37.16 | C |
| ATOM | 2697 | CD1 | LEU | S | 795 | 44.761 | 38.459 | 33.204 | 1.00 | 37.65 | C |
| ATOM | 2698 | CD2 | LEU | S | 795 | 45.450 | 40.289 | 31.718 | 1.00 | 38.07 | C |
| ATOM | 2699 | N   | THR | S | 796 | 43.936 | 35.940 | 28.796 | 1.00 | 35.47 | N |
| ATOM | 2700 | CA  | THR | S | 796 | 43.060 | 35.351 | 27.800 | 1.00 | 36.25 | C |
| ATOM | 2701 | C   | THR | S | 796 | 42.644 | 33.888 | 28.079 | 1.00 | 35.84 | C |
| ATOM | 2702 | O   | THR | S | 796 | 41.819 | 33.331 | 27.365 | 1.00 | 36.38 | O |
| ATOM | 2703 | CB  | THR | S | 796 | 43.817 | 35.429 | 26.457 | 1.00 | 36.63 | C |
| ATOM | 2704 | OG1 | THR | S | 796 | 43.251 | 34.528 | 25.524 | 1.00 | 38.48 | O |
| ATOM | 2705 | CG2 | THR | S | 796 | 45.257 | 34.907 | 26.593 | 1.00 | 37.07 | C |
| ATOM | 2706 | N   | SER | S | 797 | 43.197 | 33.251 | 29.101 | 1.00 | 35.44 | N |
| ATOM | 2707 | CA  | SER | S | 797 | 42.835 | 31.860 | 29.377 | 1.00 | 35.29 | C |
| ATOM | 2708 | C   | SER | S | 797 | 41.426 | 31.760 | 29.984 | 1.00 | 35.18 | C |
| ATOM | 2709 | O   | SER | S | 797 | 40.925 | 32.701 | 30.611 | 1.00 | 33.96 | O |
| ATOM | 2710 | CB  | SER | S | 797 | 43.856 | 31.189 | 30.291 | 1.00 | 35.17 | C |
| ATOM | 2711 | OG  | SER | S | 797 | 43.716 | 31.654 | 31.624 | 1.00 | 36.65 | O |
| ATOM | 2712 | N   | TYR | S | 798 | 40.789 | 30.611 | 29.790 | 1.00 | 35.36 | N |
| ATOM | 2713 | CA  | TYR | S | 798 | 39.427 | 30.430 | 30.256 | 1.00 | 35.94 | C |
| ATOM | 2714 | C   | TYR | S | 798 | 39.148 | 29.075 | 30.890 | 1.00 | 35.14 | C |
| ATOM | 2715 | O   | TYR | S | 798 | 39.845 | 28.095 | 30.657 | 1.00 | 35.54 | O |
| ATOM | 2716 | CB  | TYR | S | 798 | 38.440 | 30.707 | 29.120 | 1.00 | 36.37 | C |
| ATOM | 2717 | CG  | TYR | S | 798 | 38.554 | 29.794 | 27.920 | 1.00 | 39.89 | C |
| ATOM | 2718 | CD1 | TYR | S | 798 | 39.587 | 29.934 | 26.996 | 1.00 | 42.41 | C |
| ATOM | 2719 | CD2 | TYR | S | 798 | 37.606 | 28.808 | 27.697 | 1.00 | 43.13 | C |
| ATOM | 2720 | CE1 | TYR | S | 798 | 39.681 | 29.095 | 25.893 | 1.00 | 43.97 | C |
| ATOM | 2721 | CE2 | TYR | S | 798 | 37.687 | 27.963 | 26.597 | 1.00 | 44.94 | C |
| ATOM | 2722 | CZ  | TYR | S | 798 | 38.723 | 28.109 | 25.698 | 1.00 | 44.95 | C |
| ATOM | 2723 | OH  | TYR | S | 798 | 38.781 | 27.270 | 24.613 | 1.00 | 44.37 | O |
| ATOM | 2724 | N   | ASP | S | 799 | 38.108 | 29.046 | 31.709 | 1.00 | 34.54 | N |
| ATOM | 2725 | CA  | ASP | S | 799 | 37.685 | 27.840 | 32.392 | 1.00 | 33.87 | C |
| ATOM | 2726 | C   | ASP | S | 799 | 36.600 | 27.187 | 31.545 | 1.00 | 32.58 | C |
| ATOM | 2727 | O   | ASP | S | 799 | 36.465 | 27.501 | 30.366 | 1.00 | 32.32 | O |
| ATOM | 2728 | CB  | ASP | S | 799 | 37.140 | 28.208 | 33.770 | 1.00 | 34.50 | C |
| ATOM | 2729 | CG  | ASP | S | 799 | 37.299 | 27.104 | 34.773 | 1.00 | 36.07 | C |
| ATOM | 2730 | OD1 | ASP | S | 799 | 36.790 | 25.986 | 34.551 | 1.00 | 37.15 | O |
| ATOM | 2731 | OD2 | ASP | S | 799 | 37.918 | 27.279 | 35.833 | 1.00 | 41.54 | O |
| ATOM | 2732 | N   | CYS | S | 800 | 35.812 | 26.301 | 32.141 | 1.00 | 30.83 | N |
| ATOM | 2733 | CA  | CYS | S | 800 | 34.798 | 25.586 | 31.392 | 1.00 | 29.83 | C |
| ATOM | 2734 | C   | CYS | S | 800 | 33.490 | 25.511 | 32.161 | 1.00 | 29.15 | C |
| ATOM | 2735 | O   | CYS | S | 800 | 32.794 | 24.502 | 32.092 | 1.00 | 28.68 | O |
| ATOM | 2736 | CB  | CYS | S | 800 | 35.273 | 24.167 | 31.092 | 1.00 | 29.46 | C |
| ATOM | 2737 | SG  | CYS | S | 800 | 35.576 | 23.194 | 32.601 | 1.00 | 30.36 | S |
| ATOM | 2738 | N   | GLU | S | 801 | 33.152 | 26.578 | 32.874 | 1.00 | 28.36 | N |
| ATOM | 2739 | CA  | GLU | S | 801 | 31.936 | 26.605 | 33.670 | 1.00 | 28.63 | C |
| ATOM | 2740 | C   | GLU | S | 801 | 30.667 | 26.793 | 32.829 | 1.00 | 28.34 | C |
| ATOM | 2741 | O   | GLU | S | 801 | 30.626 | 27.562 | 31.867 | 1.00 | 27.30 | O |
| ATOM | 2742 | CB  | GLU | S | 801 | 32.038 | 27.688 | 34.751 | 1.00 | 28.61 | C |
| ATOM | 2743 | CG  | GLU | S | 801 | 33.252 | 27.501 | 35.655 | 1.00 | 30.83 | C |
| ATOM | 2744 | CD  | GLU | S | 801 | 33.188 | 28.346 | 36.907 | 1.00 | 32.58 | C |
| ATOM | 2745 | OE1 | GLU | S | 801 | 32.414 | 27.985 | 37.805 | 1.00 | 33.57 | O |
| ATOM | 2746 | OE2 | GLU | S | 801 | 33.910 | 29.362 | 36.989 | 1.00 | 33.97 | O |
| ATOM | 2747 | N   | VAL | S | 802 | 29.627 | 26.062 | 33.212 | 1.00 | 28.85 | N |
| ATOM | 2748 | CA  | VAL | S | 802 | 28.350 | 26.079 | 32.515 | 1.00 | 29.03 | C |
| ATOM | 2749 | C   | VAL | S | 802 | 27.233 | 26.056 | 33.546 | 1.00 | 29.80 | C |
| ATOM | 2750 | O   | VAL | S | 802 | 27.505 | 25.948 | 34.726 | 1.00 | 29.92 | O |
| ATOM | 2751 | CB  | VAL | S | 802 | 28.221 | 24.834 | 31.606 | 1.00 | 28.44 | C |
| ATOM | 2752 | CG1 | VAL | S | 802 | 29.288 | 24.856 | 30.523 | 1.00 | 26.99 | C |
| ATOM | 2753 | CG2 | VAL | S | 802 | 28.333 | 23.551 | 32.428 | 1.00 | 29.08 | C |
| ATOM | 2754 | N   | ASN | S | 803 | 25.978 | 26.135 | 33.111 | 1.00 | 31.09 | N |
| ATOM | 2755 | CA  | ASN | S | 803 | 24.853 | 26.053 | 34.042 | 1.00 | 32.53 | C |
| ATOM | 2756 | C   | ASN | S | 803 | 24.550 | 24.641 | 34.497 | 1.00 | 33.81 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2757 | O   | ASN | S | 803 | 23.456 | 24.143 | 34.270 | 1.00 | 34.27 | O |
| ATOM | 2758 | CB  | ASN | S | 803 | 23.575 | 26.659 | 33.463 | 1.00 | 32.29 | C |
| ATOM | 2759 | CG  | ASN | S | 803 | 23.640 | 28.146 | 33.367 | 1.00 | 31.77 | C |
| ATOM | 2760 | OD1 | ASN | S | 803 | 24.688 | 28.741 | 33.616 | 1.00 | 33.47 | O |
| ATOM | 2761 | ND2 | ASN | S | 803 | 22.525 | 28.772 | 33.005 | 1.00 | 29.83 | N |
| ATOM | 2762 | N   | ALA | S | 804 | 25.521 | 24.015 | 35.147 | 1.00 | 35.23 | N |
| ATOM | 2763 | CA  | ALA | S | 804 | 25.365 | 22.689 | 35.740 | 1.00 | 36.86 | C |
| ATOM | 2764 | C   | ALA | S | 804 | 26.577 | 22.452 | 36.638 | 1.00 | 37.98 | C |
| ATOM | 2765 | O   | ALA | S | 804 | 27.660 | 22.949 | 36.360 | 1.00 | 37.44 | O |
| ATOM | 2766 | CB  | ALA | S | 804 | 25.285 | 21.610 | 34.676 | 1.00 | 36.63 | C |
| ATOM | 2767 | N   | PRO | S | 805 | 26.394 | 21.694 | 37.711 | 1.00 | 40.20 | N |
| ATOM | 2768 | CA  | PRO | S | 805 | 27.495 | 21.381 | 38.635 | 1.00 | 41.46 | C |
| ATOM | 2769 | C   | PRO | S | 805 | 28.572 | 20.511 | 37.983 | 1.00 | 42.51 | C |
| ATOM | 2770 | O   | PRO | S | 805 | 28.342 | 19.931 | 36.938 | 1.00 | 43.07 | O |
| ATOM | 2771 | CB  | PRO | S | 805 | 26.799 | 20.615 | 39.774 | 1.00 | 41.54 | C |
| ATOM | 2772 | CG  | PRO | S | 805 | 25.506 | 20.116 | 39.185 | 1.00 | 41.29 | C |
| ATOM | 2773 | CD  | PRO | S | 805 | 25.117 | 21.076 | 38.115 | 1.00 | 40.40 | C |
| ATOM | 2774 | N   | ILE | S | 806 | 29.728 | 20.406 | 38.622 | 1.00 | 44.25 | N |
| ATOM | 2775 | CA  | ILE | S | 806 | 30.854 | 19.627 | 38.099 | 1.00 | 44.96 | C |
| ATOM | 2776 | C   | ILE | S | 806 | 30.770 | 18.169 | 38.532 | 1.00 | 45.18 | C |
| ATOM | 2777 | O   | ILE | S | 806 | 29.902 | 17.801 | 39.323 | 1.00 | 45.78 | O |
| ATOM | 2778 | CB  | ILE | S | 806 | 32.197 | 20.246 | 38.569 | 1.00 | 45.19 | C |
| ATOM | 2779 | CG1 | ILE | S | 806 | 32.412 | 20.018 | 40.070 | 1.00 | 46.10 | C |
| ATOM | 2780 | CG2 | ILE | S | 806 | 32.230 | 21.743 | 38.246 | 1.00 | 46.08 | C |
| ATOM | 2781 | CD1 | ILE | S | 806 | 33.740 | 20.574 | 40.597 | 1.00 | 46.98 | C |
| ATOM | 2782 | N   | LEU | S | 812 | 29.934 | 8.629  | 39.561 | 1.00 | 43.80 | N |
| ATOM | 2783 | CA  | LEU | S | 812 | 29.027 | 8.736  | 38.425 | 1.00 | 43.90 | C |
| ATOM | 2784 | C   | LEU | S | 812 | 29.761 | 9.243  | 37.182 | 1.00 | 43.45 | C |
| ATOM | 2785 | O   | LEU | S | 812 | 30.160 | 10.410 | 37.114 | 1.00 | 43.36 | O |
| ATOM | 2786 | CB  | LEU | S | 812 | 27.862 | 9.678  | 38.757 | 1.00 | 44.22 | C |
| ATOM | 2787 | CG  | LEU | S | 812 | 26.979 | 9.292  | 39.951 | 1.00 | 45.50 | C |
| ATOM | 2788 | CD1 | LEU | S | 812 | 25.871 | 10.341 | 40.144 | 1.00 | 46.20 | C |
| ATOM | 2789 | CD2 | LEU | S | 812 | 26.385 | 7.894  | 39.793 | 1.00 | 45.08 | C |
| ATOM | 2790 | N   | LEU | S | 813 | 29.928 | 8.375  | 36.190 | 1.00 | 42.70 | N |
| ATOM | 2791 | CA  | LEU | S | 813 | 30.620 | 8.776  | 34.969 | 1.00 | 42.21 | C |
| ATOM | 2792 | C   | LEU | S | 813 | 29.711 | 9.604  | 34.057 | 1.00 | 41.46 | C |
| ATOM | 2793 | O   | LEU | S | 813 | 28.492 | 9.438  | 34.062 | 1.00 | 41.23 | O |
| ATOM | 2794 | CB  | LEU | S | 813 | 31.167 | 7.554  | 34.225 | 1.00 | 42.30 | C |
| ATOM | 2795 | CG  | LEU | S | 813 | 32.093 | 6.644  | 35.046 | 1.00 | 42.35 | C |
| ATOM | 2796 | CD1 | LEU | S | 813 | 32.494 | 5.419  | 34.233 | 1.00 | 42.48 | C |
| ATOM | 2797 | CD2 | LEU | S | 813 | 33.322 | 7.398  | 35.527 | 1.00 | 41.80 | C |
| ATOM | 2798 | N   | GLN | S | 814 | 30.326 | 10.492 | 33.283 | 1.00 | 40.74 | N |
| ATOM | 2799 | CA  | GLN | S | 814 | 29.603 | 11.385 | 32.378 | 1.00 | 40.26 | C |
| ATOM | 2800 | C   | GLN | S | 814 | 30.475 | 11.775 | 31.190 | 1.00 | 39.82 | C |
| ATOM | 2801 | O   | GLN | S | 814 | 31.674 | 11.514 | 31.176 | 1.00 | 39.19 | O |
| ATOM | 2802 | CB  | GLN | S | 814 | 29.173 | 12.649 | 33.122 | 1.00 | 40.24 | C |
| ATOM | 2803 | CG  | GLN | S | 814 | 30.336 | 13.501 | 33.615 | 1.00 | 40.51 | C |
| ATOM | 2804 | CD  | GLN | S | 814 | 29.879 | 14.725 | 34.406 | 1.00 | 41.88 | C |
| ATOM | 2805 | OE1 | GLN | S | 814 | 29.200 | 14.590 | 35.419 | 1.00 | 41.86 | O |
| ATOM | 2806 | NE2 | GLN | S | 814 | 30.253 | 15.919 | 33.940 | 1.00 | 40.63 | N |
| ATOM | 2807 | N   | GLY | S | 815 | 29.864 | 12.416 | 30.200 | 1.00 | 39.81 | N |
| ATOM | 2808 | CA  | GLY | S | 815 | 30.568 | 12.851 | 29.012 | 1.00 | 39.53 | C |
| ATOM | 2809 | C   | GLY | S | 815 | 31.402 | 11.755 | 28.365 | 1.00 | 39.85 | C |
| ATOM | 2810 | O   | GLY | S | 815 | 30.962 | 10.609 | 28.210 | 1.00 | 38.55 | O |
| ATOM | 2811 | N   | GLU | S | 816 | 32.624 | 12.123 | 27.995 | 1.00 | 40.44 | N |
| ATOM | 2812 | CA  | GLU | S | 816 | 33.553 | 11.208 | 27.352 | 1.00 | 41.24 | C |
| ATOM | 2813 | C   | GLU | S | 816 | 33.744 | 9.926  | 28.154 | 1.00 | 41.73 | C |
| ATOM | 2814 | O   | GLU | S | 816 | 33.895 | 8.852  | 27.577 | 1.00 | 41.11 | O |
| ATOM | 2815 | CB  | GLU | S | 816 | 34.909 | 11.884 | 27.148 | 1.00 | 41.24 | C |
| ATOM | 2816 | CG  | GLU | S | 816 | 35.752 | 11.238 | 26.063 | 1.00 | 42.19 | C |
| ATOM | 2817 | CD  | GLU | S | 816 | 37.161 | 11.790 | 26.019 | 1.00 | 43.70 | C |

|        |      |     |     |       |     |        |        |        |      |       |    |
|--------|------|-----|-----|-------|-----|--------|--------|--------|------|-------|----|
| ATOM   | 2818 | OE1 | GLU | S     | 816 | 37.985 | 11.311 | 26.814 | 1.00 | 45.25 | O  |
| ATOM   | 2819 | OE2 | GLU | S     | 816 | 37.447 | 12.696 | 25.201 | 1.00 | 44.50 | O  |
| ATOM   | 2820 | N   | GLU | S     | 817 | 33.724 | 10.039 | 29.479 | 1.00 | 42.66 | N  |
| ATOM   | 2821 | CA  | GLU | S     | 817 | 33.925 | 8.877  | 30.340 | 1.00 | 43.73 | C  |
| ATOM   | 2822 | C   | GLU | S     | 817 | 32.744 | 7.917  | 30.268 | 1.00 | 44.19 | C  |
| ATOM   | 2823 | O   | GLU | S     | 817 | 32.930 | 6.699  | 30.252 | 1.00 | 43.99 | O  |
| ATOM   | 2824 | CB  | GLU | S     | 817 | 34.167 | 9.308  | 31.788 | 1.00 | 43.81 | C  |
| ATOM   | 2825 | CG  | GLU | S     | 817 | 35.463 | 10.077 | 31.989 | 1.00 | 44.98 | C  |
| ATOM   | 2826 | CD  | GLU | S     | 817 | 35.337 | 11.569 | 31.688 | 1.00 | 46.95 | C  |
| ATOM   | 2827 | OE1 | GLU | S     | 817 | 34.221 | 12.052 | 31.394 | 1.00 | 48.87 | O  |
| ATOM   | 2828 | OE2 | GLU | S     | 817 | 36.362 | 12.277 | 31.748 | 1.00 | 49.02 | O  |
| ATOM   | 2829 | N   | LEU | S     | 818 | 31.536 | 8.470  | 30.231 | 1.00 | 44.93 | N  |
| ATOM   | 2830 | CA  | LEU | S     | 818 | 30.335 | 7.663  | 30.149 | 1.00 | 45.78 | C  |
| ATOM   | 2831 | C   | LEU | S     | 818 | 30.359 | 6.882  | 28.846 | 1.00 | 46.89 | C  |
| ATOM   | 2832 | O   | LEU | S     | 818 | 30.163 | 5.663  | 28.833 | 1.00 | 46.50 | O  |
| ATOM   | 2833 | CB  | LEU | S     | 818 | 29.077 | 8.537  | 30.219 | 1.00 | 45.65 | C  |
| ATOM   | 2834 | CG  | LEU | S     | 818 | 27.741 | 7.788  | 30.147 | 1.00 | 45.58 | C  |
| ATOM   | 2835 | CD1 | LEU | S     | 818 | 27.612 | 6.809  | 31.318 | 1.00 | 45.36 | C  |
| ATOM   | 2836 | CD2 | LEU | S     | 818 | 26.551 | 8.719  | 30.133 | 1.00 | 43.95 | C  |
| ATOM   | 2837 | N   | LEU | S     | 819 | 30.654 | 7.588  | 27.760 | 1.00 | 48.01 | N  |
| ATOM   | 2838 | CA  | LEU | S     | 819 | 30.607 | 7.014  | 26.420 | 1.00 | 49.24 | C  |
| ATOM   | 2839 | C   | LEU | S     | 819 | 31.559 | 5.829  | 26.247 | 1.00 | 50.32 | C  |
| ATOM   | 2840 | O   | LEU | S     | 819 | 31.169 | 4.777  | 25.731 | 1.00 | 50.11 | O  |
| ATOM   | 2841 | CB  | LEU | S     | 819 | 30.903 | 8.105  | 25.380 | 1.00 | 49.22 | C  |
| ATOM   | 2842 | CG  | LEU | S     | 819 | 30.848 | 7.724  | 23.901 | 1.00 | 49.32 | C  |
| ATOM   | 2843 | CD1 | LEU | S     | 819 | 29.495 | 7.178  | 23.497 | 1.00 | 48.73 | C  |
| ATOM   | 2844 | CD2 | LEU | S     | 819 | 31.205 | 8.940  | 23.058 | 1.00 | 49.85 | C  |
| ATOM   | 2845 | N   | ARG | S     | 820 | 32.801 | 6.005  | 26.684 | 1.00 | 51.33 | N  |
| ATOM   | 2846 | CA  | ARG | S     | 820 | 33.807 | 4.966  | 26.550 | 1.00 | 52.53 | C  |
| ATOM   | 2847 | C   | ARG | S     | 820 | 33.471 | 3.748  | 27.414 | 1.00 | 52.95 | C  |
| ATOM   | 2848 | O   | ARG | S     | 820 | 33.534 | 2.606  | 26.942 | 1.00 | 53.06 | O  |
| ATOM   | 2849 | CB  | ARG | S     | 820 | 35.185 | 5.529  | 26.898 | 1.00 | 52.91 | C  |
| ATOM   | 2850 | CG  | ARG | S     | 820 | 35.620 | 6.583  | 25.904 | 1.00 | 54.20 | C  |
| ATOM   | 2851 | CD  | ARG | S     | 820 | 37.044 | 7.046  | 26.040 | 1.00 | 55.94 | C  |
| ATOM   | 2852 | NE  | ARG | S     | 820 | 37.320 | 8.113  | 25.081 | 1.00 | 58.09 | N  |
| ATOM   | 2853 | CZ  | ARG | S     | 820 | 38.453 | 8.808  | 25.022 | 1.00 | 59.82 | C  |
| ATOM   | 2854 | NH1 | ARG | S     | 820 | 39.448 | 8.555  | 25.867 | 1.00 | 60.28 | N  |
| ATOM   | 2855 | NH2 | ARG | S     | 820 | 38.590 | 9.765  | 24.108 | 1.00 | 60.61 | N  |
| ATOM   | 2856 | N   | ALA | S     | 821 | 33.106 | 3.994  | 28.670 | 1.00 | 53.36 | N  |
| ATOM   | 2857 | CA  | ALA | S     | 821 | 32.698 | 2.920  | 29.561 | 1.00 | 53.67 | C  |
| ATOM   | 2858 | C   | ALA | S     | 821 | 31.598 | 2.094  | 28.892 | 1.00 | 54.08 | C  |
| ATOM   | 2859 | O   | ALA | S     | 821 | 31.648 | 0.862  | 28.897 | 1.00 | 54.01 | O  |
| ATOM   | 2860 | CB  | ALA | S     | 821 | 32.215 | 3.479  | 30.883 | 1.00 | 53.55 | C  |
| ATOM   | 2861 | N   | LEU | S     | 822 | 30.616 | 2.777  | 28.308 | 1.00 | 54.44 | N  |
| ATOM   | 2862 | CA  | LEU | S     | 822 | 29.516 | 2.110  | 27.622 | 1.00 | 54.93 | C  |
| ATOM   | 2863 | C   | LEU | S     | 822 | 30.007 | 1.342  | 26.398 | 1.00 | 55.41 | C  |
| ATOM   | 2864 | O   | LEU | S     | 822 | 29.557 | 0.230  | 26.143 | 1.00 | 55.60 | O  |
| ATOM   | 2865 | CB  | LEU | S     | 822 | 28.445 | 3.117  | 27.212 | 1.00 | 54.90 | C  |
| ATOM   | 2866 | CG  | LEU | S     | 822 | 27.667 | 3.756  | 28.361 | 1.00 | 54.80 | C  |
| ATOM   | 2867 | CD1 | LEU | S     | 822 | 26.531 | 4.601  | 27.801 | 1.00 | 54.39 | C  |
| ATOM   | 2868 | CD2 | LEU | S     | 822 | 27.139 | 2.702  | 29.335 | 1.00 | 54.48 | C  |
| ATOM   | 2869 | N   | ASP | S     | 823 | 30.911 | 1.949  | 25.634 | 1.00 | 55.82 | N  |
| ATOM   | 2870 | CA  | ASP | S     | 823 | 31.525 | 1.282  | 24.492 | 1.00 | 56.04 | C  |
| ATOM   | 2871 | C   | ASP | S     | 823 | 32.893 | 0.735  | 24.901 | 1.00 | 56.10 | C  |
| ATOM   | 2872 | O   | ASP | S     | 823 | 33.186 | -0.451 | 24.731 | 1.00 | 56.09 | O  |
| ATOM   | 2873 | CB  | ASP | S     | 823 | 31.688 | 2.252  | 23.320 | 1.00 | 56.21 | C  |
| ATOM   | 2874 | CG  | ASP | S     | 823 | 31.858 | 1.535  | 21.997 | 1.00 | 56.45 | C  |
| ATOM   | 2875 | OD1 | ASP | S     | 823 | 32.245 | 0.351  | 22.028 | 1.00 | 58.65 | O  |
| ATOM   | 2876 | OD2 | ASP | S     | 823 | 31.628 | 2.056  | 20.885 | 1.00 | 56.19 | O  |
| TER    | 2877 |     | ASP | S     | 823 |        |        |        |      |       |    |
| HETATM | 2878 | FE  | FE2 | A1350 |     | 23.294 | 27.501 | 28.594 | 1.00 | 20.46 | FE |

|        |      |    |     |       |        |        |        |      |       |   |
|--------|------|----|-----|-------|--------|--------|--------|------|-------|---|
| HETATM | 2879 | C1 | OGA | A1351 | 22.091 | 25.173 | 27.594 | 1.00 | 24.79 | C |
| HETATM | 2880 | C2 | OGA | A1351 | 21.066 | 25.829 | 28.202 | 1.00 | 24.27 | C |
| HETATM | 2881 | C4 | OGA | A1351 | 18.756 | 25.714 | 29.004 | 1.00 | 23.09 | C |
| HETATM | 2882 | C5 | OGA | A1351 | 17.415 | 25.241 | 28.495 | 1.00 | 23.17 | C |
| HETATM | 2883 | O1 | OGA | A1351 | 21.909 | 24.061 | 27.090 | 1.00 | 25.24 | O |
| HETATM | 2884 | O2 | OGA | A1351 | 23.219 | 25.658 | 27.531 | 1.00 | 24.40 | O |
| HETATM | 2885 | O2 | OGA | A1351 | 21.192 | 26.959 | 28.711 | 1.00 | 21.19 | O |
| HETATM | 2886 | O3 | OGA | A1351 | 16.416 | 25.662 | 29.055 | 1.00 | 23.03 | O |
| HETATM | 2887 | N1 | OGA | A1351 | 19.886 | 25.203 | 28.228 | 1.00 | 21.70 | N |
| HETATM | 2888 | O4 | OGA | A1351 | 17.332 | 24.475 | 27.537 | 1.00 | 23.98 | O |
| HETATM | 2889 | S  | SO4 | A1352 | 0.316  | 25.182 | 43.602 | 1.00 | 77.77 | S |
| HETATM | 2890 | O1 | SO4 | A1352 | 1.239  | 25.980 | 44.403 | 1.00 | 77.64 | O |
| HETATM | 2891 | O2 | SO4 | A1352 | 1.075  | 24.260 | 42.760 | 1.00 | 77.88 | O |
| HETATM | 2892 | O3 | SO4 | A1352 | -0.525 | 24.416 | 44.514 | 1.00 | 78.38 | O |
| HETATM | 2893 | O4 | SO4 | A1352 | -0.507 | 26.042 | 42.757 | 1.00 | 76.90 | O |
| HETATM | 2894 | S  | SO4 | A1353 | 1.990  | 28.487 | 29.834 | 1.00 | 69.20 | S |
| HETATM | 2895 | O1 | SO4 | A1353 | 3.243  | 29.065 | 30.309 | 1.00 | 68.34 | O |
| HETATM | 2896 | O2 | SO4 | A1353 | 2.236  | 27.438 | 28.847 | 1.00 | 67.90 | O |
| HETATM | 2897 | O3 | SO4 | A1353 | 1.298  | 27.948 | 31.009 | 1.00 | 70.32 | O |
| HETATM | 2898 | O4 | SO4 | A1353 | 1.162  | 29.517 | 29.203 | 1.00 | 69.63 | O |
| HETATM | 2899 | O  | HOH | H 1   | 35.955 | 31.618 | 40.285 | 1.00 | 80.01 | O |
| HETATM | 2900 | O  | HOH | H 2   | 38.513 | 33.804 | 31.613 | 1.00 | 33.04 | O |
| HETATM | 2901 | O  | HOH | H 3   | 36.648 | 25.786 | 38.779 | 1.00 | 76.96 | O |
| HETATM | 2902 | O  | HOH | H 4   | 38.106 | 25.337 | 29.179 | 1.00 | 54.79 | O |
| HETATM | 2903 | O  | HOH | H 5   | 34.990 | 30.561 | 34.967 | 1.00 | 30.13 | O |
| HETATM | 2904 | O  | HOH | H 6   | 33.934 | 31.237 | 38.711 | 1.00 | 40.66 | O |
| HETATM | 2905 | O  | HOH | H 7   | 30.766 | 25.787 | 37.613 | 1.00 | 54.75 | O |
| HETATM | 2906 | O  | HOH | H 8   | 33.667 | 28.867 | 40.196 | 1.00 | 59.66 | O |
| HETATM | 2907 | O  | HOH | H 9   | 28.622 | 27.043 | 37.556 | 1.00 | 57.58 | O |
| HETATM | 2908 | O  | HOH | H 10  | 19.894 | 26.655 | 33.706 | 1.00 | 54.88 | O |
| HETATM | 2909 | O  | HOH | H 11  | 30.052 | 24.213 | 35.628 | 1.00 | 41.23 | O |
| HETATM | 2910 | O  | HOH | H 12  | 28.737 | 12.960 | 37.083 | 1.00 | 59.80 | O |
| HETATM | 2911 | O  | HOH | H 13  | 35.568 | 13.822 | 23.888 | 1.00 | 38.00 | O |
| HETATM | 2912 | O  | HOH | H 14  | 30.722 | -1.323 | 21.296 | 1.00 | 48.92 | O |
| HETATM | 2913 | O  | HOH | H 15  | 32.110 | 2.136  | 17.673 | 1.00 | 69.92 | O |
| HETATM | 2914 | O  | HOH | Z 1   | 9.466  | 21.720 | 12.039 | 1.00 | 63.79 | O |
| HETATM | 2915 | O  | HOH | Z 2   | 1.367  | 21.270 | 7.724  | 1.00 | 60.01 | O |
| HETATM | 2916 | O  | HOH | Z 3   | 3.426  | 13.325 | 8.811  | 1.00 | 43.04 | O |
| HETATM | 2917 | O  | HOH | Z 4   | -0.760 | 13.029 | 7.574  | 1.00 | 47.08 | O |
| HETATM | 2918 | O  | HOH | Z 5   | 2.515  | 19.304 | 5.195  | 1.00 | 46.76 | O |
| HETATM | 2919 | O  | HOH | Z 6   | 4.861  | 33.534 | 13.331 | 1.00 | 75.60 | O |
| HETATM | 2920 | O  | HOH | Z 7   | 1.403  | 29.250 | 13.007 | 1.00 | 46.80 | O |
| HETATM | 2921 | O  | HOH | Z 8   | 1.614  | 32.100 | 13.758 | 1.00 | 66.18 | O |
| HETATM | 2922 | O  | HOH | Z 9   | 12.671 | 34.540 | 13.968 | 1.00 | 43.83 | O |
| HETATM | 2923 | O  | HOH | Z 10  | 11.399 | 2.867  | 17.750 | 1.00 | 68.06 | O |
| HETATM | 2924 | O  | HOH | Z 11  | -1.220 | 30.205 | 22.820 | 1.00 | 80.54 | O |
| HETATM | 2925 | O  | HOH | Z 12  | 6.576  | 36.529 | 29.511 | 1.00 | 43.88 | O |
| HETATM | 2926 | O  | HOH | Z 13  | 3.525  | 32.513 | 31.866 | 1.00 | 65.87 | O |
| HETATM | 2927 | O  | HOH | Z 14  | 5.033  | 37.447 | 27.566 | 1.00 | 54.03 | O |
| HETATM | 2928 | O  | HOH | Z 15  | 10.981 | 35.615 | 30.196 | 1.00 | 36.24 | O |
| HETATM | 2929 | O  | HOH | Z 16  | 12.816 | 42.461 | 26.787 | 1.00 | 37.83 | O |
| HETATM | 2930 | O  | HOH | Z 17  | 13.508 | 37.138 | 13.905 | 1.00 | 50.79 | O |
| HETATM | 2931 | O  | HOH | Z 18  | 16.409 | 3.305  | 16.425 | 1.00 | 59.87 | O |
| HETATM | 2932 | O  | HOH | Z 19  | 14.424 | 4.598  | 17.530 | 1.00 | 54.39 | O |
| HETATM | 2933 | O  | HOH | Z 20  | 11.439 | 7.927  | 15.708 | 1.00 | 63.10 | O |
| HETATM | 2934 | O  | HOH | Z 21  | 15.821 | 30.360 | 12.573 | 1.00 | 43.61 | O |
| HETATM | 2935 | O  | HOH | Z 22  | 13.496 | 22.189 | 7.246  | 1.00 | 57.93 | O |
| HETATM | 2936 | O  | HOH | Z 23  | 17.591 | 29.863 | 7.160  | 1.00 | 49.97 | O |
| HETATM | 2937 | O  | HOH | Z 24  | 14.617 | 26.200 | 13.898 | 1.00 | 48.56 | O |
| HETATM | 2938 | O  | HOH | Z 25  | 20.840 | 23.785 | 3.695  | 1.00 | 38.79 | O |
| HETATM | 2939 | O  | HOH | Z 26  | 27.946 | 19.151 | 9.101  | 1.00 | 43.14 | O |



|        |      |   |     |   |    |        |        |        |      |       |   |
|--------|------|---|-----|---|----|--------|--------|--------|------|-------|---|
| HETATM | 2940 | O | HOH | Z | 27 | 23.279 | 21.788 | 0.672  | 1.00 | 62.23 | O |
| HETATM | 2941 | O | HOH | Z | 28 | 27.443 | 22.009 | 43.177 | 1.00 | 68.81 | O |
| HETATM | 2942 | O | HOH | Z | 29 | 27.326 | 30.900 | 5.769  | 1.00 | 84.31 | O |
| HETATM | 2943 | O | HOH | Z | 30 | 16.938 | 35.662 | 41.749 | 1.00 | 51.88 | O |
| HETATM | 2944 | O | HOH | Z | 31 | 36.792 | 29.262 | 21.033 | 1.00 | 42.38 | O |
| HETATM | 2945 | O | HOH | Z | 32 | 26.719 | 37.403 | 13.167 | 1.00 | 60.20 | O |
| HETATM | 2946 | O | HOH | Z | 33 | 29.797 | 37.021 | 10.379 | 1.00 | 60.24 | O |
| HETATM | 2947 | O | HOH | Z | 34 | 28.365 | 37.713 | 15.023 | 1.00 | 68.08 | O |
| HETATM | 2948 | O | HOH | Z | 35 | 27.471 | 34.815 | 9.298  | 1.00 | 63.90 | O |
| HETATM | 2949 | O | HOH | Z | 36 | 24.262 | 32.919 | 12.792 | 1.00 | 45.02 | O |
| HETATM | 2950 | O | HOH | Z | 37 | 19.704 | 17.909 | 13.178 | 1.00 | 28.78 | O |
| HETATM | 2951 | O | HOH | Z | 38 | 22.022 | 12.870 | 8.792  | 1.00 | 48.37 | O |
| HETATM | 2952 | O | HOH | Z | 39 | 18.151 | 14.971 | 12.982 | 1.00 | 36.76 | O |
| HETATM | 2953 | O | HOH | Z | 40 | 29.160 | 5.439  | 16.977 | 1.00 | 44.05 | O |
| HETATM | 2954 | O | HOH | Z | 41 | 18.863 | 14.590 | 16.204 | 1.00 | 30.84 | O |
| HETATM | 2955 | O | HOH | Z | 42 | 12.149 | 5.293  | 13.385 | 1.00 | 72.13 | O |
| HETATM | 2956 | O | HOH | Z | 43 | 15.651 | 2.782  | 13.845 | 1.00 | 41.52 | O |
| HETATM | 2957 | O | HOH | Z | 44 | 14.014 | 7.467  | 18.234 | 1.00 | 52.22 | O |
| HETATM | 2958 | O | HOH | Z | 45 | 5.548  | 12.548 | 27.846 | 1.00 | 38.03 | O |
| HETATM | 2959 | O | HOH | Z | 46 | 12.742 | 5.782  | 36.187 | 1.00 | 51.07 | O |
| HETATM | 2960 | O | HOH | Z | 47 | 19.063 | 6.567  | 36.600 | 1.00 | 49.16 | O |
| HETATM | 2961 | O | HOH | Z | 48 | 19.545 | 2.633  | 38.104 | 1.00 | 67.28 | O |
| HETATM | 2962 | O | HOH | Z | 49 | 7.710  | 14.276 | 19.473 | 1.00 | 48.41 | O |
| HETATM | 2963 | O | HOH | Z | 50 | 15.732 | 7.234  | 38.833 | 1.00 | 54.12 | O |
| HETATM | 2964 | O | HOH | Z | 51 | 21.932 | 13.291 | 44.351 | 1.00 | 62.49 | O |
| HETATM | 2965 | O | HOH | Z | 52 | 33.998 | 44.086 | 25.334 | 1.00 | 53.56 | O |
| HETATM | 2966 | O | HOH | Z | 53 | 12.673 | 21.178 | 43.612 | 1.00 | 63.01 | O |
| HETATM | 2967 | O | HOH | Z | 54 | 8.172  | 26.738 | 44.107 | 1.00 | 61.46 | O |
| HETATM | 2968 | O | HOH | Z | 55 | 9.613  | 30.854 | 42.520 | 1.00 | 54.56 | O |
| HETATM | 2969 | O | HOH | Z | 56 | 13.563 | 35.806 | 31.131 | 1.00 | 39.09 | O |
| HETATM | 2970 | O | HOH | Z | 57 | 15.688 | 37.473 | 35.304 | 1.00 | 47.58 | O |
| HETATM | 2971 | O | HOH | Z | 58 | 7.422  | 43.868 | 25.982 | 1.00 | 75.57 | O |
| HETATM | 2972 | O | HOH | Z | 59 | 7.978  | 38.223 | 34.865 | 1.00 | 59.51 | O |
| HETATM | 2973 | O | HOH | Z | 60 | 16.338 | 30.836 | 40.223 | 1.00 | 38.80 | O |
| HETATM | 2974 | O | HOH | Z | 61 | 17.035 | 27.760 | 38.288 | 1.00 | 52.22 | O |
| HETATM | 2975 | O | HOH | Z | 62 | 22.131 | 25.023 | 41.390 | 1.00 | 55.16 | O |
| HETATM | 2976 | O | HOH | Z | 63 | 29.869 | 29.910 | 39.122 | 1.00 | 47.28 | O |
| HETATM | 2977 | O | HOH | Z | 64 | 28.353 | 24.399 | 41.766 | 1.00 | 60.35 | O |
| HETATM | 2978 | O | HOH | Z | 65 | 31.794 | 27.570 | 41.962 | 1.00 | 48.59 | O |
| HETATM | 2979 | O | HOH | Z | 66 | 28.058 | 28.695 | 48.927 | 1.00 | 65.95 | O |
| HETATM | 2980 | O | HOH | Z | 67 | 24.838 | 24.783 | 42.190 | 1.00 | 52.90 | O |
| HETATM | 2981 | O | HOH | Z | 68 | 11.541 | 32.183 | 15.082 | 1.00 | 63.99 | O |
| HETATM | 2982 | O | HOH | Z | 69 | 31.599 | 33.767 | 45.823 | 1.00 | 44.28 | O |
| HETATM | 2983 | O | HOH | Z | 70 | 24.728 | 38.721 | 49.282 | 1.00 | 48.25 | O |
| HETATM | 2984 | O | HOH | Z | 71 | 16.271 | 36.399 | 44.087 | 1.00 | 58.46 | O |
| HETATM | 2985 | O | HOH | Z | 72 | 17.845 | 37.716 | 46.244 | 1.00 | 57.93 | O |
| HETATM | 2986 | O | HOH | Z | 73 | 16.480 | 33.117 | 41.520 | 1.00 | 59.15 | O |
| HETATM | 2987 | O | HOH | Z | 74 | 40.791 | 21.415 | 26.920 | 1.00 | 58.98 | O |
| HETATM | 2988 | O | HOH | Z | 75 | 21.842 | 17.819 | 48.106 | 1.00 | 67.11 | O |
| HETATM | 2989 | O | HOH | Z | 76 | 8.791  | 17.468 | 46.626 | 1.00 | 63.28 | O |
| HETATM | 2990 | O | HOH | Z | 77 | 17.141 | 16.914 | 47.607 | 1.00 | 52.87 | O |
| HETATM | 2991 | O | HOH | Z | 78 | 21.626 | 14.804 | 40.702 | 1.00 | 53.91 | O |
| HETATM | 2992 | O | HOH | Z | 79 | 39.117 | 50.091 | 47.735 | 1.00 | 57.17 | O |
| HETATM | 2993 | O | HOH | Z | 80 | 10.617 | 19.257 | 44.587 | 1.00 | 69.00 | O |
| HETATM | 2994 | O | HOH | Z | 81 | 1.682  | 24.435 | 36.842 | 1.00 | 55.40 | O |
| HETATM | 2995 | O | HOH | Z | 82 | 4.627  | 30.781 | 36.487 | 1.00 | 53.38 | O |
| HETATM | 2996 | O | HOH | Z | 83 | 17.463 | 26.906 | 33.818 | 1.00 | 38.64 | O |
| HETATM | 2997 | O | HOH | Z | 84 | 18.429 | 25.785 | 36.464 | 1.00 | 54.65 | O |
| HETATM | 2998 | O | HOH | Z | 85 | 23.466 | 17.336 | 36.578 | 1.00 | 41.94 | O |
| HETATM | 2999 | O | HOH | Z | 86 | 26.890 | 12.949 | 30.365 | 1.00 | 49.34 | O |
| HETATM | 3000 | O | HOH | Z | 87 | 21.694 | 10.405 | 34.333 | 1.00 | 45.95 | O |



|        |      |   |     |   |     |        |        |        |      |       |   |
|--------|------|---|-----|---|-----|--------|--------|--------|------|-------|---|
| HETATM | 3001 | O | HOH | Z | 88  | 20.030 | 9.589  | 36.847 | 1.00 | 52.33 | O |
| HETATM | 3002 | O | HOH | Z | 89  | 18.447 | -1.706 | 32.981 | 1.00 | 66.29 | O |
| HETATM | 3003 | O | HOH | Z | 90  | 16.300 | -0.205 | 30.017 | 1.00 | 50.70 | O |
| HETATM | 3004 | O | HOH | Z | 91  | 17.950 | 1.645  | 20.589 | 1.00 | 51.55 | O |
| HETATM | 3005 | O | HOH | Z | 92  | 26.301 | 5.439  | 16.918 | 1.00 | 36.67 | O |
| HETATM | 3006 | O | HOH | Z | 93  | 33.944 | 10.218 | 13.383 | 1.00 | 51.60 | O |
| HETATM | 3007 | O | HOH | Z | 94  | 30.893 | 16.371 | 11.174 | 1.00 | 40.00 | O |
| HETATM | 3008 | O | HOH | Z | 95  | 32.606 | 13.689 | 20.709 | 1.00 | 45.01 | O |
| HETATM | 3009 | O | HOH | Z | 96  | 31.860 | 10.158 | 7.765  | 1.00 | 58.55 | O |
| HETATM | 3010 | O | HOH | Z | 97  | 36.957 | 10.422 | 7.614  | 1.00 | 76.91 | O |
| HETATM | 3011 | O | HOH | Z | 98  | 35.951 | 16.836 | 31.735 | 1.00 | 59.28 | O |
| HETATM | 3012 | O | HOH | Z | 99  | 39.867 | 18.412 | 27.150 | 1.00 | 50.38 | O |
| HETATM | 3013 | O | HOH | Z | 100 | 13.436 | 20.952 | 28.355 | 1.00 | 27.89 | O |
| HETATM | 3014 | O | HOH | Z | 101 | 3.992  | 21.265 | 30.540 | 1.00 | 43.76 | O |
| HETATM | 3015 | O | HOH | Z | 102 | 30.735 | 37.910 | 33.103 | 1.00 | 30.45 | O |
| HETATM | 3016 | O | HOH | Z | 103 | 25.986 | 26.303 | 26.047 | 1.00 | 26.08 | O |
| HETATM | 3017 | O | HOH | Z | 104 | 36.837 | 32.025 | 33.001 | 1.00 | 37.86 | O |
| HETATM | 3018 | O | HOH | Z | 105 | 35.845 | 25.360 | 27.653 | 1.00 | 33.53 | O |
| HETATM | 3019 | O | HOH | Z | 106 | 31.874 | 20.474 | 33.040 | 1.00 | 55.47 | O |
| HETATM | 3020 | O | HOH | Z | 107 | 36.793 | 26.619 | 20.918 | 1.00 | 34.57 | O |
| HETATM | 3021 | O | HOH | Z | 108 | 17.114 | 16.909 | 17.862 | 1.00 | 35.83 | O |
| HETATM | 3022 | O | HOH | Z | 109 | 9.968  | 13.510 | 19.464 | 1.00 | 37.10 | O |
| HETATM | 3023 | O | HOH | Z | 110 | 5.274  | 16.717 | 22.023 | 1.00 | 44.26 | O |
| HETATM | 3024 | O | HOH | Z | 111 | 7.041  | 16.862 | 20.149 | 1.00 | 37.71 | O |
| HETATM | 3025 | O | HOH | Z | 112 | 6.517  | 22.763 | 22.963 | 1.00 | 38.94 | O |
| HETATM | 3026 | O | HOH | Z | 113 | 29.471 | 38.812 | 26.249 | 1.00 | 22.19 | O |
| HETATM | 3027 | O | HOH | Z | 114 | 32.253 | 43.121 | 24.229 | 1.00 | 53.95 | O |
| HETATM | 3028 | O | HOH | Z | 115 | 28.797 | 40.227 | 16.136 | 1.00 | 64.15 | O |
| HETATM | 3029 | O | HOH | Z | 116 | 30.645 | 39.042 | 18.925 | 1.00 | 33.21 | O |
| HETATM | 3030 | O | HOH | Z | 117 | 25.466 | 42.302 | 17.883 | 1.00 | 64.00 | O |
| HETATM | 3031 | O | HOH | Z | 118 | 27.698 | 44.486 | 31.068 | 1.00 | 26.13 | O |
| HETATM | 3032 | O | HOH | Z | 119 | 30.274 | 44.879 | 25.031 | 1.00 | 38.32 | O |
| HETATM | 3033 | O | HOH | Z | 120 | 27.635 | 48.525 | 29.776 | 1.00 | 35.59 | O |
| HETATM | 3034 | O | HOH | Z | 121 | 25.933 | 50.527 | 30.463 | 1.00 | 35.79 | O |
| HETATM | 3035 | O | HOH | Z | 122 | 26.614 | 31.094 | 38.158 | 1.00 | 32.11 | O |
| HETATM | 3036 | O | HOH | Z | 123 | 29.486 | 36.934 | 35.226 | 1.00 | 27.40 | O |
| HETATM | 3037 | O | HOH | Z | 124 | 30.510 | 30.229 | 36.300 | 1.00 | 31.99 | O |
| HETATM | 3038 | O | HOH | Z | 125 | 19.859 | 31.575 | 33.786 | 1.00 | 31.77 | O |
| HETATM | 3039 | O | HOH | Z | 126 | 18.490 | 38.301 | 36.415 | 1.00 | 43.54 | O |
| HETATM | 3040 | O | HOH | Z | 127 | 19.538 | 36.155 | 33.217 | 1.00 | 30.91 | O |
| HETATM | 3041 | O | HOH | Z | 128 | 25.386 | 44.358 | 40.124 | 1.00 | 54.33 | O |
| HETATM | 3042 | O | HOH | Z | 129 | 21.227 | 42.704 | 39.938 | 1.00 | 38.88 | O |
| HETATM | 3043 | O | HOH | Z | 130 | 17.603 | 37.763 | 31.961 | 1.00 | 35.39 | O |
| HETATM | 3044 | O | HOH | Z | 131 | 9.290  | 41.007 | 35.589 | 1.00 | 51.53 | O |
| HETATM | 3045 | O | HOH | Z | 132 | 9.348  | 43.374 | 27.752 | 1.00 | 61.17 | O |
| HETATM | 3046 | O | HOH | Z | 133 | 15.089 | 37.816 | 32.481 | 1.00 | 32.05 | O |
| HETATM | 3047 | O | HOH | Z | 134 | 10.824 | 48.278 | 31.295 | 1.00 | 52.52 | O |
| HETATM | 3048 | O | HOH | Z | 135 | 15.691 | 44.668 | 34.824 | 1.00 | 31.47 | O |
| HETATM | 3049 | O | HOH | Z | 136 | 15.962 | 46.870 | 38.981 | 1.00 | 51.42 | O |
| HETATM | 3050 | O | HOH | Z | 137 | 13.481 | 51.613 | 32.894 | 1.00 | 45.77 | O |
| HETATM | 3051 | O | HOH | Z | 138 | 14.202 | 48.658 | 24.558 | 1.00 | 43.59 | O |
| HETATM | 3052 | O | HOH | Z | 139 | 16.193 | 44.497 | 37.574 | 1.00 | 58.87 | O |
| HETATM | 3053 | O | HOH | Z | 140 | 15.573 | 46.265 | 24.419 | 1.00 | 39.51 | O |
| HETATM | 3054 | O | HOH | Z | 141 | 18.684 | 55.873 | 28.304 | 1.00 | 58.28 | O |
| HETATM | 3055 | O | HOH | Z | 142 | 14.817 | 55.477 | 27.388 | 1.00 | 52.87 | O |
| HETATM | 3056 | O | HOH | Z | 143 | 15.284 | 50.258 | 22.000 | 1.00 | 32.96 | O |
| HETATM | 3057 | O | HOH | Z | 144 | 23.651 | 46.151 | 19.718 | 1.00 | 33.04 | O |
| HETATM | 3058 | O | HOH | Z | 145 | 16.751 | 46.565 | 21.800 | 1.00 | 33.97 | O |
| HETATM | 3059 | O | HOH | Z | 146 | 12.595 | 29.171 | 13.536 | 1.00 | 39.79 | O |
| HETATM | 3060 | O | HOH | Z | 147 | 10.812 | 19.188 | 14.084 | 1.00 | 50.88 | O |
| HETATM | 3061 | O | HOH | Z | 148 | 11.495 | 21.508 | 13.792 | 1.00 | 44.23 | O |

[illegible]

Structure 2

Below are the coordinates for structure 2 (the 2.25 Å structure of FIH:Fe(II):2OG:CAD):

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HEADER      TRANSCRIPTION ACTIVATOR/INHIBITOR          12-AUG-02   1H2L
TITLE       FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE       2 FRAGMENT PEPTIDE
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND      3 CHAIN: A;
COMPND      4 ENGINEERED: YES;
COMPND      5 MOL_ID: 2;
COMPND      6 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND      7 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
COMPND      8 MEMBER OF PAS PROTEIN 1;
COMPND      9 CHAIN: S;
COMPND     10 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND     11 RESIDUES 786-826
SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE      3 ORGANISM_COMMON: HUMAN;
SOURCE      4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE      5 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE      6 EXPRESSION_SYSTEM_PLASMID: PET28A(+);
SOURCE      7 MOL_ID: 2;
SOURCE      8 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE      9 ORGANISM_COMMON: HUMAN;
SOURCE     10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE     11 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE     12 EXPRESSION_SYSTEM_PLASMID: PGEX-GP-1
KEYWDS      FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
KEYWDS      2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE
EXPDTA      X-RAY DIFFRACTION
AUTHOR      J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,I.SCHLEMMINGER,
AUTHOR      2 J.F.SEIBEL,C.J.SCHOFIELD
REVDAT      1   04-SEP-02 1H2L   0
JRNL        AUTH   J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,
JRNL        AUTH 2 I.SCHLEMMINGER,J.F.SEIBEL,C.J.SCHOFIELD
JRNL        TITL   FIH:HIF-FRAGMENT COMPLEXES
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK      2
REMARK      2 RESOLUTION. 2.25 ANGSTROMS.
REMARK      3
REMARK      3 REFINEMENT.
REMARK      3   PROGRAM       : REFMAC 5.0
REMARK      3   AUTHORS        : MURSHUDOV,VAGIN,DODSON
REMARK      3
REMARK      3   REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK      3
REMARK      3 DATA USED IN REFINEMENT.
REMARK      3   RESOLUTION RANGE HIGH (ANGSTROMS) :   2.25
REMARK      3   RESOLUTION RANGE LOW  (ANGSTROMS)  :  38.00
REMARK      3   DATA CUTOFF          (SIGMA(F))      : NONE
REMARK      3   COMPLETENESS FOR RANGE               (%) :  99.98
REMARK      3   NUMBER OF REFLECTIONS                  :  25127
REMARK      3
REMARK      3 FIT TO DATA USED IN REFINEMENT.
REMARK      3   CROSS-VALIDATION METHOD                      : THROUGHOUT

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REMARK 3   FREE R VALUE TEST SET SELECTION   : RANDOM
REMARK 3   R VALUE      (WORKING + TEST SET) : 0.18514
REMARK 3   R VALUE      (WORKING SET)       : 0.18253
REMARK 3   FREE R VALUE                               : 0.21738
REMARK 3   FREE R VALUE TEST SET SIZE    (%) : 7.7
REMARK 3   FREE R VALUE TEST SET COUNT    : 2104
REMARK 3
REMARK 3   FIT IN THE HIGHEST RESOLUTION BIN.
REMARK 3   TOTAL NUMBER OF BINS USED           :      20
REMARK 3   BIN RESOLUTION RANGE HIGH          :    2.250
REMARK 3   BIN RESOLUTION RANGE LOW           :    2.308
REMARK 3   REFLECTION IN BIN      (WORKING SET) :    1783
REMARK 3   BIN R VALUE      (WORKING SET)      :    0.194
REMARK 3   BIN FREE R VALUE SET COUNT         :    170
REMARK 3   BIN FREE R VALUE                   :    0.228
REMARK 3
REMARK 3   NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3   PROTEIN ATOMS                      : 2863
REMARK 3   NUCLEIC ACID ATOMS                  : 0
REMARK 3   HETEROGEN ATOMS                    : 21
REMARK 3   SOLVENT ATOMS                      : 139
REMARK 3
REMARK 3   B VALUES.
REMARK 3   FROM WILSON PLOT                     (A**2) : NULL
REMARK 3   MEAN B VALUE      (OVERALL, A**2)    : 27.234
REMARK 3   OVERALL ANISOTROPIC B VALUE.
REMARK 3   B11 (A**2) :    -0.40
REMARK 3   B22 (A**2) :    -0.40
REMARK 3   B33 (A**2) :     0.80
REMARK 3   B12 (A**2) :     0.00
REMARK 3   B13 (A**2) :     0.00
REMARK 3   B23 (A**2) :     0.00
REMARK 3
REMARK 3   ESTIMATED OVERALL COORDINATE ERROR.
REMARK 3   ESU BASED ON R VALUE                      (A): 0.203
REMARK 3   ESU BASED ON FREE R VALUE                  (A): 0.174
REMARK 3   ESU BASED ON MAXIMUM LIKELIHOOD            (A): 0.165
REMARK 3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 6.444
REMARK 3
REMARK 3   CORRELATION COEFFICIENTS.
REMARK 3   CORRELATION COEFFICIENT FO-FC              : 0.956
REMARK 3   CORRELATION COEFFICIENT FO-FC FREE         : 0.939
REMARK 3
REMARK 3   RMS DEVIATIONS FROM IDEAL VALUES      COUNT      RMS      WEIGHT
REMARK 3   BOND LENGTHS REFINED                      (A): 2961 ; 0.013 ; 0.021
REMARK 3   BOND LENGTHS REFINED                      (A): 2961 ; 0.013 ; 0.021
REMARK 3   BOND LENGTHS OTHERS                        (A): 2554 ; 0.001 ; 0.020
REMARK 3   BOND ANGLES REFINED      (DEGREES): 4026 ; 1.404 ; 1.949
REMARK 3   BOND ANGLES OTHERS      (DEGREES): 5966 ; 0.727 ; 3.000
REMARK 3   TORSION ANGLES, PERIOD 1 (DEGREES): 350 ; 4.037 ; 3.000
REMARK 3   TORSION ANGLES, PERIOD 3 (DEGREES): 515 ; 18.189 ; 15.000
REMARK 3   CHIRAL-CENTER RESTRAINTS      (A**3): 413 ; 0.085 ; 0.200
REMARK 3   GENERAL PLANES REFINED          (A): 3315 ; 0.005 ; 0.020
REMARK 3   GENERAL PLANES OTHERS           (A): 602 ; 0.002 ; 0.020
REMARK 3   NON-BONDED CONTACTS REFINED      (A): 693 ; 0.221 ; 0.300
REMARK 3   NON-BONDED CONTACTS OTHERS      (A): 2483 ; 0.204 ; 0.300
REMARK 3   H-BOND (X...Y) REFINED          (A): 208 ; 0.156 ; 0.500
REMARK 3   SYMMETRY VDW REFINED            (A): 16 ; 0.256 ; 0.300
REMARK 3   SYMMETRY VDW OTHERS            (A): 63 ; 0.259 ; 0.300
REMARK 3   SYMMETRY H-BOND REFINED        (A): 10 ; 0.200 ; 0.500
REMARK 3

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REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS. COUNT RMS WEIGHT  
REMARK 3 MAIN-CHAIN BOND REFINED (A\*\*2): 1767 ; 0.649 ; 1.500  
REMARK 3 MAIN-CHAIN ANGLE REFINED (A\*\*2): 2847 ; 1.227 ; 2.000  
REMARK 3 SIDE-CHAIN BOND REFINED (A\*\*2): 1194 ; 1.887 ; 3.000  
REMARK 3 SIDE-CHAIN ANGLE REFINED (A\*\*2): 1179 ; 3.111 ; 4.500  
REMARK 3  
REMARK 3 NCS RESTRAINTS STATISTICS  
REMARK 3 NUMBER OF NCS GROUPS : NULL  
REMARK 3  
REMARK 3 TLS DETAILS  
REMARK 3 NUMBER OF TLS GROUPS : 1  
REMARK 3  
REMARK 3 TLS GROUP : 1  
REMARK 3 NUMBER OF COMPONENTS GROUP : 2  
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI  
REMARK 3 RESIDUE RANGE : A 15 A 451  
REMARK 3 RESIDUE RANGE : S 795 S 822  
REMARK 3 ORIGIN FOR THE GROUP (A): 22.2240 27.6230 28.5830  
REMARK 3 T TENSOR  
REMARK 3 T11: 0.1744 T22: 0.0216  
REMARK 3 T33: 0.0949 T12: -0.0059  
REMARK 3 T13: -0.0546 T23: 0.0427  
REMARK 3 L TENSOR  
REMARK 3 L11: 1.1183 L22: 2.4664  
REMARK 3 L33: 1.3415 L12: 0.7934  
REMARK 3 L13: 0.5409 L23: 1.2249  
REMARK 3 S TENSOR  
REMARK 3 S11: 0.0358 S12: -0.1772 S13: -0.0521  
REMARK 3 S21: 0.1763 S22: 0.0025 S23: 0.1089  
REMARK 3 S31: 0.2114 S32: -0.0339 S33: -0.0383  
REMARK 3  
REMARK 3 BULK SOLVENT MODELLING.  
REMARK 3 METHOD USED : BABINET MODEL WITH MASK  
REMARK 3 PARAMETERS FOR MASK CALCULATION  
REMARK 3 VDW PROBE RADIUS : 1.40  
REMARK 3 ION PROBE RADIUS : 0.80  
REMARK 3 SHRINKAGE RADIUS : 0.80  
REMARK 3  
REMARK 3 OTHER REFINEMENT REMARKS: HYDROGENS HAVE BEEN ADDED IN THE  
REMARK 3 RIDING POSITIONS  
REMARK 4  
REMARK 4 1H2L COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998  
REMARK 100  
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.  
REMARK 100 THE EBI ID CODE IS EBI-11172.  
REMARK 200  
REMARK 200 EXPERIMENTAL DETAILS  
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION  
REMARK 200 DATE OF DATA COLLECTION : 15-MAY-2002  
REMARK 200 TEMPERATURE (KELVIN) : 100  
REMARK 200 PH : 7.5  
REMARK 200 NUMBER OF CRYSTALS USED : 1  
REMARK 200  
REMARK 200 SYNCHROTRON (Y/N) : Y  
REMARK 200 RADIATION SOURCE : SRS BEAMLINE PX14.2  
REMARK 200 BEAMLINE : PX14.2  
REMARK 200 X-RAY GENERATOR MODEL : NULL  
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M  
REMARK 200 WAVELENGTH OR RANGE (A) : 0.983  
REMARK 200 MONOCHROMATOR : NULL  
REMARK 200 OPTICS : NULL

REMARK 200  
REMARK 200 DETECTOR TYPE : CCD  
REMARK 200 DETECTOR MANUFACTURER : ADSC  
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : MOSFLM  
REMARK 200 DATA SCALING SOFTWARE : SCALA  
REMARK 200  
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 27294  
REMARK 200 RESOLUTION RANGE HIGH (A) : 2.25  
REMARK 200 RESOLUTION RANGE LOW (A) : 38.63  
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NONE  
REMARK 200  
REMARK 200 OVERALL.  
REMARK 200 COMPLETENESS FOR RANGE (%) : 100.0  
REMARK 200 DATA REDUNDANCY : 7.0  
REMARK 200 R MERGE (I) : 0.058  
REMARK 200 R SYM (I) : NULL  
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 9.7  
REMARK 200  
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.  
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.25  
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A) : 2.37  
REMARK 200 COMPLETENESS FOR SHELL (%) : 100.0  
REMARK 200 DATA REDUNDANCY IN SHELL : 7.2  
REMARK 200 R MERGE FOR SHELL (I) : 0.307  
REMARK 200 R SYM FOR SHELL (I) : NULL  
REMARK 200 <I/SIGMA(I)> FOR SHELL : 2.5  
REMARK 200  
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH  
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT  
REMARK 200 SOFTWARE USED: NULL  
REMARK 200 STARTING MODEL: NULL  
REMARK 200  
REMARK 200 REMARK: NULL  
REMARK 280  
REMARK 280 CRYSTAL  
REMARK 280 SOLVENT CONTENT, VS (%): 63  
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS\*\*3/DA): 3.4  
REMARK 280  
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE, 4% PEG400,  
REMARK 280 0.1M HEPES PH7.5, ARGON ATMOSPHERE, 11MG/ML PROTEIN WITH  
REMARK 280 1MM FE(II), 2.5MM AKG AND 2.5MM PEPTIDE  
REMARK 290  
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY  
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2  
REMARK 290  
REMARK 290 SYMOP SYMMETRY  
REMARK 290 NNNMMM OPERATOR  
REMARK 290 1555 X, Y, Z  
REMARK 290 2555 -X, -Y, 1/2+Z  
REMARK 290 3555 1/2-Y, 1/2+X, 1/4+Z  
REMARK 290 4555 1/2+Y, 1/2-X, 3/4+Z  
REMARK 290 5555 1/2-X, 1/2+Y, 1/4-Z  
REMARK 290 6555 1/2+X, 1/2-Y, 3/4-Z  
REMARK 290 7555 Y, X, -Z  
REMARK 290 8555 -Y, -X, 1/2-Z  
REMARK 290  
REMARK 290 WHERE NNN -> OPERATOR NUMBER  
REMARK 290 MMM -> TRANSLATION VECTOR  
REMARK 290  
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS  
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM

REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY  
REMARK 290 RELATED MOLECULES.

|            |        |   |           |           |           |           |
|------------|--------|---|-----------|-----------|-----------|-----------|
| REMARK 290 | SMTRY1 | 1 | 1.000000  | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 1 | 0.000000  | 1.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 1 | 0.000000  | 0.000000  | 1.000000  | 0.000000  |
| REMARK 290 | SMTRY1 | 2 | -1.000000 | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 2 | 0.000000  | -1.000000 | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 2 | 0.000000  | 0.000000  | 1.000000  | 73.95700  |
| REMARK 290 | SMTRY1 | 3 | 0.000000  | -1.000000 | 0.000000  | 43.13200  |
| REMARK 290 | SMTRY2 | 3 | 1.000000  | 0.000000  | 0.000000  | 43.13200  |
| REMARK 290 | SMTRY3 | 3 | 0.000000  | 0.000000  | 1.000000  | 36.97850  |
| REMARK 290 | SMTRY1 | 4 | 0.000000  | 1.000000  | 0.000000  | 43.13200  |
| REMARK 290 | SMTRY2 | 4 | -1.000000 | 0.000000  | 0.000000  | 43.13200  |
| REMARK 290 | SMTRY3 | 4 | 0.000000  | 0.000000  | 1.000000  | 110.93550 |
| REMARK 290 | SMTRY1 | 5 | -1.000000 | 0.000000  | 0.000000  | 43.13200  |
| REMARK 290 | SMTRY2 | 5 | 0.000000  | 1.000000  | 0.000000  | 43.13200  |
| REMARK 290 | SMTRY3 | 5 | 0.000000  | 0.000000  | -1.000000 | 36.97850  |
| REMARK 290 | SMTRY1 | 6 | 1.000000  | 0.000000  | 0.000000  | 43.13200  |
| REMARK 290 | SMTRY2 | 6 | 0.000000  | -1.000000 | 0.000000  | 43.13200  |
| REMARK 290 | SMTRY3 | 6 | 0.000000  | 0.000000  | -1.000000 | 110.93550 |
| REMARK 290 | SMTRY1 | 7 | 0.000000  | 1.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 7 | 1.000000  | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 7 | 0.000000  | 0.000000  | -1.000000 | 0.000000  |
| REMARK 290 | SMTRY1 | 8 | 0.000000  | -1.000000 | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 8 | -1.000000 | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 8 | 0.000000  | 0.000000  | -1.000000 | 73.95700  |

REMARK 290  
REMARK 290 REMARK: NULL  
REMARK 300  
REMARK 300 BIOMOLECULE: 1  
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT  
REMARK 300 WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR  
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).  
REMARK 300  
REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC  
REMARK 300  
REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.  
REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S  
REMARK 300 PRODUCES A TETRAMER.  
REMARK 300  
REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE  
REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT  
REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE  
REMARK 300 HOMODIMER OF CHAIN A  
REMARK 300  
REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS  
REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH  
REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER  
REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR  
REMARK 300 THE CHAIN IN THE COMPLEX IS 2141.3 ANGSTROM\*\*2  
REMARK 350  
REMARK 350 GENERATING THE BIOMOLECULE  
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN  
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE  
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS  
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND  
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.  
REMARK 350  
REMARK 350 BIOMOLECULE: 1  
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S  
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 0.000000

REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000 0.000000  
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000 0.000000  
REMARK 350 BIOMT1 2 0.000000 -1.000000 0.000000 86.26400  
REMARK 350 BIOMT2 2 -1.000000 0.000000 0.000000 86.26400  
REMARK 350 BIOMT3 2 0.000000 0.000000 -1.000000 73.95700

REMARK 465

REMARK 465 MISSING RESIDUES

REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE

REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN

REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)

REMARK 465

REMARK 465 M RES C SSSEQI

REMARK 465 MET A 1

REMARK 465 ALA A 2

REMARK 465 ALA A 3

REMARK 465 THR A 4

REMARK 465 ALA A 5

REMARK 465 ALA A 6

REMARK 465 GLU A 7

REMARK 465 ALA A 8

REMARK 465 VAL A 9

REMARK 465 ALA A 10

REMARK 465 SER A 11

REMARK 465 GLY A 12

REMARK 465 SER A 13

REMARK 465 GLY A 14

REMARK 465 LYS A 304

REMARK 465 ARG A 305

REMARK 465 ILE A 306

REMARK 465 SER S 786

REMARK 465 MET S 787

REMARK 465 ASP S 788

REMARK 465 GLU S 789

REMARK 465 SER S 790

REMARK 465 GLY S 791

REMARK 465 LEU S 792

REMARK 465 PRO S 793

REMARK 465 GLN S 794

REMARK 465 GLN S 807

REMARK 465 GLY S 808

REMARK 465 SER S 809

REMARK 465 ARG S 810

REMARK 465 ASN S 811

REMARK 465 LEU S 812

REMARK 465 ASP S 823

REMARK 465 GLN S 824

REMARK 465 VAL S 825

REMARK 465 ASN S 826

REMARK 470

REMARK 470 MISSING ATOM

REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;

REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;

REMARK 470 I=INSERTION CODE):

REMARK 470 M RES CSSEQI ATOMS

REMARK 470 GLU A 15 CG CD OE1 OE2

REMARK 470 GLU A 29 CG CD OE1 OE2

REMARK 470 ASN A 87 CG OD1 ND2

REMARK 470 LYS A 106 CD CE NZ

REMARK 470 ARG A 117 CG CD NE CZ NH1 NH2

REMARK 470 GLN A 133 CG CD OE1 NE2

REMARK 470 GLN A 136 CG CD OE1 NE2



REMARK 470 GLN A 137 CG CD OE1 NE2  
 REMARK 470 ARG A 156 CG CD NE CZ NH1 NH2  
 REMARK 470 LYS A 157 CD CE NZ  
 REMARK 470 LYS A 311 CG CD CE NZ  
 REMARK 500  
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY  
 REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS  
 REMARK 500  
 REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES  
 REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE  
 REMARK 500 THAN 6\*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL  
 REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE  
 REMARK 500 NUMBER; I=INSERTION CODE).  
 REMARK 500  
 REMARK 500 STANDARD TABLE:  
 REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,1X,2(A4,A1,3X),12X,F5.3)  
 REMARK 500  
 REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991  
 REMARK 500  

| M | RES | CSSEQI | ATM1 | RES | CSSEQI | ATM2  | DEVIATION |
|---|-----|--------|------|-----|--------|-------|-----------|
|   | MET | A      | 343  | SD  | MET    | A 343 | CE -0.243 |

 REMARK 500  
 REMARK 500 REMARK: NULL  
 REMARK 500  
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY  
 REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT  
 REMARK 500  
 REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.  
 REMARK 500  

| ATM1 | RES | C | SSEQI | ATM2 | RES | C | SSEQI | DISTANCE |
|------|-----|---|-------|------|-----|---|-------|----------|
| O    | ALA | A | 300   | OH   | TYR | S | 798   | 2.18     |

 REMARK 500  
 REMARK 525  
 REMARK 525 SOLVENT  
 REMARK 525  
 REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO  
 REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY  
 REMARK 525 ASSOCIATED WITH:  

| PROTEIN CHAIN | SOLVENT CHAIN |
|---------------|---------------|
| A             | Z             |
| S             | H             |

 REMARK 525  
 REMARK 600  
 REMARK 600 HETEROGEN  
 REMARK 600  
 REMARK 600 FOR METAL ATOM FE FE2 A1350 THE COORDINATION ANGLES ARE:  

|                | 1     | 2     | 3    | 4    |
|----------------|-------|-------|------|------|
| 1 HIS 199A NE2 |       |       |      |      |
| 2 ASP 201A OD2 | 103.4 |       |      |      |
| 3 HIS 279A NE2 | 83.1  | 86.0  |      |      |
| 4 AKG 1351A O1 | 168.9 | 87.6  | 98.2 |      |
| 5 AKG 1351A O5 | 87.0  | 169.4 | 97.2 | 81.9 |

 REMARK 600  
 REMARK 700  
 REMARK 700 SHEET  
 REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN  
 REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,  
 REMARK 700 TWO SHEETS ARE DEFINED.  
 REMARK 800  
 REMARK 800 SITE  
 REMARK 800 SITE\_IDENTIFIER: FE1  
 REMARK 800 SITE\_DESCRIPTION: FE BINDING SITE FOR CHAIN A  
 REMARK 800

REMARK 800 SITE\_IDENTIFIER: AKG  
 REMARK 800 SITE\_DESCRIPTION: AKG BINDING SITE FOR CHAIN A  
 REMARK 800  
 REMARK 800 SITE\_IDENTIFIER: SO1  
 REMARK 800 SITE\_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A  
 REMARK 800  
 REMARK 800 SITE\_IDENTIFIER: SO2  
 REMARK 800 SITE\_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A  
 REMARK 900

REMARK 900 RELATED ENTRIES

REMARK 900 RELATED ID: 1D7G RELATED DB: PDB  
 REMARK 900 A MODEL FOR THE COMPLEX BETWEEN THE  
 REMARK 900 HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS  
 REMARK 900 CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE  
 REMARK 900 RELATED ID: 1H2K RELATED DB: PDB  
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX  
 REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE  
 REMARK 900 RELATED ID: 1H2M RELATED DB: PDB  
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX  
 REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE  
 REMARK 900 RELATED ID: 1H2N RELATED DB: PDB  
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX  
 REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE  
 REMARK 900 RELATED ID: 1L8C RELATED DB: PDB  
 REMARK 900 STRUCTURAL BASIS FOR HIF-1ALPHA/CBP  
 REMARK 900 RECOGNITION IN THECELLULAR HYPOXIC RESPONSE  
 REMARK 900 RELATED ID: 1LM8 RELATED DB: PDB  
 REMARK 900 STRUCTURE OF A HIF-1A-PVHL-ELONGINB-  
 REMARK 900 ELONGINC COMPLEX  
 REMARK 900 RELATED ID: 1LQB RELATED DB: PDB  
 REMARK 900 CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1  
 REMARK 900 ALPHA PEPTIDEBOUND TO THE PVHL/ELONGIN-C/  
 REMARK 900 ELONGIN-B COMPLEX

|        |      |   |     |     |     |        |            |     |     |
|--------|------|---|-----|-----|-----|--------|------------|-----|-----|
| DBREF  | 1H2L | A | 1   | 349 | SWS | Q969Q7 | Q969Q7     | 1   | 349 |
| DBREF  | 1H2L | S | 786 | 826 | SWS | Q16665 | HIFA_HUMAN | 786 | 826 |
| SEQRES | 1    | A | 349 | MET | ALA | ALA    | THR        | ALA | ALA |
| SEQRES | 2    | A | 349 | GLY | GLU | PRO    | ARG        | GLU | GLU |
| SEQRES | 3    | A | 349 | TRP | ASP | GLU    | SER        | GLN | LEU |
| SEQRES | 4    | A | 349 | ARG | PRO | ILE    | PRO        | ARG | LEU |
| SEQRES | 5    | A | 349 | GLU | GLU | LEU    | ILE        | GLU | ASN |
| SEQRES | 6    | A | 349 | ASP | THR | ASN    | LEU        | VAL | TYR |
| SEQRES | 7    | A | 349 | GLU | TYR | LEU    | GLN        | GLU | ASN |
| SEQRES | 8    | A | 349 | VAL | TYR | SER    | ALA        | SER | THR |
| SEQRES | 9    | A | 349 | GLU | LYS | LYS    | MET        | ALA | ASN |
| SEQRES | 10   | A | 349 | SER | ASN | ARG    | GLU        | GLU | MET |
| SEQRES | 11   | A | 349 | LYS | LEU | GLN    | ASP        | ILE | GLN |
| SEQRES | 12   | A | 349 | LEU | TYR | LEU    | GLN        | GLN | THR |
| SEQRES | 13   | A | 349 | LYS | ILE | VAL    | MET        | ASP | PHE |
| SEQRES | 14   | A | 349 | ILE | ASN | LYS    | GLN        | GLN | GLY |
| SEQRES | 15   | A | 349 | THR | SER | ASN    | LEU        | LEU | ILE |
| SEQRES | 16   | A | 349 | THR | PRO | ALA    | HIS        | TYR | ASP |
| SEQRES | 17   | A | 349 | GLN | ILE | LYS    | GLY        | TYR | LYS |
| SEQRES | 18   | A | 349 | ASP | GLN | PHE    | GLU        | CYS | LEU |
| SEQRES | 19   | A | 349 | PRO | CYS | ASP    | ARG        | GLN | SER |
| SEQRES | 20   | A | 349 | ASP | TYR | GLU    | ARG        | PHE | PRO |
| SEQRES | 21   | A | 349 | TYR | GLU | THR    | VAL        | VAL | GLY |
| SEQRES | 22   | A | 349 | PRO | MET | TYR    | TRP        | TRP | HIS |
| SEQRES | 23   | A | 349 | GLY | GLY | ILE    | THR        | ILE | THR |
| SEQRES | 24   | A | 349 | ALA | PRO | THR    | PRO        | LYS | ARG |
| SEQRES | 25   | A | 349 | HIS | GLN | LYS    | VAL        | ALA | ILE |
| SEQRES | 26   | A | 349 | LEU | GLY | GLU    | ALA        | LEU | GLY |

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SEQRES  27 A  349  LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN
SEQRES   1 S   41  SER MET ASP GLU SER GLY LEU PRO GLN LEU THR SER TYR
SEQRES   2 S   41  ASP CYS GLU VAL ASN ALA PRO ILE GLN GLY SER ARG ASN
SEQRES   3 S   41  LEU LEU GLN GLY GLU GLU LEU LEU ARG ALA LEU ASP GLN
SEQRES   4 S   41  VAL ASN
HET      FE2  A1350      1
HET      AKG  A1351     10
HET      SO4  A1352      5
HET      SO4  A1353      5
HETNAM      FE2 FE (II) ION
HETNAM      AKG 2-OXYGLUTARIC ACID
HETNAM      SO4 SULFATE ION
FORMUL      3  FE2      FE1 2+
FORMUL      4  AKG      C5 H6 O5
FORMUL      5  SO4      2(O4 S1 2-)
FORMUL      6  HOH      *139(H2 O1)
HELIX       1    1 ASP A    28  LEU A    32  5
HELIX       2    2 ASP A    49  ASN A    58  1
HELIX       3    3 VAL A    70  TRP A    76  5
HELIX       4    4 ASP A    77  ILE A    85  1
HELIX       5    5 ASP A   104  PHE A   111  5
HELIX       6    6 LYS A   124  ARG A   138  1
HELIX       7    7 GLY A   155  GLY A   164  1
HELIX       8    8 ASN A   166  GLY A   178  1
HELIX       9    9 PRO A   220  ASP A   222  5
HELIX      10   10 GLN A   223  TYR A   228  1
HELIX      11   11 PHE A   252  VAL A   258  5
HELIX      12   12 LYS A   311  GLY A   331  1
HELIX      13   13 ASN A   332  GLN A   334  5
HELIX      14   14 GLU A   335  LYS A   345  1
HELIX      15   15 GLN S   814  LEU S   822  1
SHEET       1  AA 5 THR A    39  PRO A    41  0
SHEET       2  AA 5 GLY A   260  VAL A   265  1 O GLY A   260  N ARG A    40
SHEET       3  AA 5 LYS A   214  PHE A   219 -1 O LYS A   214  N VAL A   265
SHEET       4  AA 5 TRP A   278  SER A   283 -1 O TRP A   278  N PHE A   219
SHEET       5  AA 5 VAL A   195  HIS A   199 -1 O THR A   196  N ILE A   281
SHEET       1  AB 6 ARG A    44  LEU A    45  0
SHEET       2  AB 6 VAL A    62  LEU A    64  1 O VAL A    63  N LEU A    45
SHEET       3  AB 6 VAL A   270  ILE A   273 -1 O VAL A   270  N LEU A    64
SHEET       4  AB 6 GLN A   204  LYS A   211 -1 O ASN A   205  N ILE A   273
SHEET       5  AB 6 THR A   290  TYR A   297 -1 O ILE A   291  N ILE A   210
SHEET       6  AB 6 LEU A   182  SER A   184 -1 N THR A   183  O TRP A   296
SHEET       1  AC 9 ARG A    44  LEU A    45  0
SHEET       2  AC 9 VAL A    62  LEU A    64  1 O VAL A    63  N LEU A    45
SHEET       3  AC 9 VAL A   270  ILE A   273 -1 O VAL A   270  N LEU A    64
SHEET       4  AC 9 GLN A   204  LYS A   211 -1 O ASN A   205  N ILE A   273
SHEET       5  AC 9 THR A   290  TYR A   297 -1 O ILE A   291  N ILE A   210
SHEET       6  AC 9 LEU A   186  GLY A   190 -1 O LEU A   186  N ASN A   294
SHEET       7  AC 9 ARG A   143  THR A   149 -1 O LEU A   146  N ILE A   189
SHEET       8  AC 9 PHE A    90  ALA A    95 -1 O SER A    91  N GLN A   147
SHEET       9  AC 9 SER A   118  MET A   123 -1 O ASN A   119  N SER A    94
LINK         FE  FE2 A1350      NE2 HIS A   199      1555      1555
LINK         FE  FE2 A1350      OD2 ASP A   201      1555      1555
LINK         FE  FE2 A1350      NE2 HIS A   279      1555      1555
LINK         FE  FE2 A1350      O1  AKG A1351      1555      1555
LINK         FE  FE2 A1350      O5  AKG A1351      1555      1555
CISPEP      1  TYR A   308      PRO A   309      0      1.27
SITE        1  FE1   3  HIS A   199  ASP A   201  HIS A   279
SITE        1  AKG  12  TYR A   145  THR A   196  HIS A   199  ASP A   201
SITE        2  AKG  12  ASN A   205  PHE A   207  LYS A   214  HIS A   279
SITE        3  AKG  12  ILE A   281  ASN A   294  TRP A   296  HOH Z    65

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|        |          |     |          |     |          |     |        |        |       |        |          |       |     |    |     |   |
|--------|----------|-----|----------|-----|----------|-----|--------|--------|-------|--------|----------|-------|-----|----|-----|---|
| SITE   | 1        | SO1 | 4        | ARG | A        | 138 | GLY    | A      | 140   | GLU    | A        | 141   | GLU | A  | 142 |   |
| SITE   | 1        | SO2 | 5        | ARG | A        | 143 | GLU    | A      | 192   | GLY    | A        | 193   | LEU | A  | 285 |   |
| SITE   | 2        | SO2 | 5        | ASN | A        | 286 |        |        |       |        |          |       |     |    |     |   |
| CRYST1 | 86.264   |     | 86.264   |     | 147.914  |     | 90.00  |        | 90.00 |        | 90.00    | P     | 41  | 21 | 2   | 8 |
| ORIGX1 | 1.000000 |     | 0.000000 |     | 0.000000 |     |        |        |       |        | 0.000000 |       |     |    |     |   |
| ORIGX2 | 0.000000 |     | 1.000000 |     | 0.000000 |     |        |        |       |        | 0.000000 |       |     |    |     |   |
| ORIGX3 | 0.000000 |     | 0.000000 |     | 1.000000 |     |        |        |       |        | 0.000000 |       |     |    |     |   |
| SCALE1 | 0.011592 |     | 0.000000 |     | 0.000000 |     |        |        |       |        | 0.000000 |       |     |    |     |   |
| SCALE2 | 0.000000 |     | 0.011592 |     | 0.000000 |     |        |        |       |        | 0.000000 |       |     |    |     |   |
| SCALE3 | 0.000000 |     | 0.000000 |     | 0.006761 |     |        |        |       |        | 0.000000 |       |     |    |     |   |
| ATOM   | 1        | N   |          | GLU | A        | 15  | 8.505  | 32.866 |       | 9.893  | 1.00     | 61.72 |     |    |     | N |
| ATOM   | 2        | CA  |          | GLU | A        | 15  | 7.173  | 32.223 |       | 9.682  | 1.00     | 61.95 |     |    |     | C |
| ATOM   | 3        | C   |          | GLU | A        | 15  | 7.251  | 30.749 |       | 10.070 | 1.00     | 61.54 |     |    |     | C |
| ATOM   | 4        | O   |          | GLU | A        | 15  | 8.109  | 30.026 |       | 9.581  | 1.00     | 61.66 |     |    |     | O |
| ATOM   | 5        | CB  |          | GLU | A        | 15  | 6.724  | 32.375 |       | 8.234  | 1.00     | 62.08 |     |    |     | C |
| ATOM   | 6        | N   |          | PRO | A        | 16  | 6.353  | 30.305 |       | 10.941 | 1.00     | 61.24 |     |    |     | N |
| ATOM   | 7        | CA  |          | PRO | A        | 16  | 6.386  | 28.928 |       | 11.455 | 1.00     | 60.97 |     |    |     | C |
| ATOM   | 8        | C   |          | PRO | A        | 16  | 6.342  | 27.853 |       | 10.368 | 1.00     | 60.27 |     |    |     | C |
| ATOM   | 9        | O   |          | PRO | A        | 16  | 5.494  | 27.879 |       | 9.479  | 1.00     | 60.01 |     |    |     | O |
| ATOM   | 10       | CB  |          | PRO | A        | 16  | 5.134  | 28.849 |       | 12.333 | 1.00     | 61.10 |     |    |     | C |
| ATOM   | 11       | CG  |          | PRO | A        | 16  | 4.790  | 30.262 |       | 12.653 | 1.00     | 61.53 |     |    |     | C |
| ATOM   | 12       | CD  |          | PRO | A        | 16  | 5.228  | 31.079 |       | 11.488 | 1.00     | 61.35 |     |    |     | C |
| ATOM   | 13       | N   |          | ARG | A        | 17  | 7.256  | 26.900 |       | 10.464 | 1.00     | 59.45 |     |    |     | N |
| ATOM   | 14       | CA  |          | ARG | A        | 17  | 7.348  | 25.820 |       | 9.494  | 1.00     | 59.05 |     |    |     | C |
| ATOM   | 15       | C   |          | ARG | A        | 17  | 6.083  | 24.971 |       | 9.478  | 1.00     | 57.86 |     |    |     | C |
| ATOM   | 16       | O   |          | ARG | A        | 17  | 5.312  | 24.963 |       | 10.437 | 1.00     | 57.86 |     |    |     | O |
| ATOM   | 17       | CB  |          | ARG | A        | 17  | 8.541  | 24.913 |       | 9.827  | 1.00     | 59.53 |     |    |     | C |
| ATOM   | 18       | CG  |          | ARG | A        | 17  | 9.906  | 25.621 |       | 9.859  | 1.00     | 60.69 |     |    |     | C |
| ATOM   | 19       | CD  |          | ARG | A        | 17  | 11.080 | 24.696 |       | 10.194 | 1.00     | 62.32 |     |    |     | C |
| ATOM   | 20       | NE  |          | ARG | A        | 17  | 11.040 | 24.185 |       | 11.567 | 1.00     | 63.73 |     |    |     | N |
| ATOM   | 21       | CZ  |          | ARG | A        | 17  | 11.464 | 24.852 |       | 12.649 | 1.00     | 65.28 |     |    |     | C |
| ATOM   | 22       | NH1 |          | ARG | A        | 17  | 11.962 | 26.085 |       | 12.544 | 1.00     | 65.01 |     |    |     | N |
| ATOM   | 23       | NH2 |          | ARG | A        | 17  | 11.385 | 24.282 |       | 13.848 | 1.00     | 65.09 |     |    |     | N |
| ATOM   | 24       | N   |          | GLU | A        | 18  | 5.878  | 24.254 |       | 8.382  | 1.00     | 56.26 |     |    |     | N |
| ATOM   | 25       | CA  |          | GLU | A        | 18  | 4.749  | 23.351 |       | 8.273  | 1.00     | 55.12 |     |    |     | C |
| ATOM   | 26       | C   |          | GLU | A        | 18  | 5.222  | 21.931 |       | 8.587  | 1.00     | 53.54 |     |    |     | C |
| ATOM   | 27       | O   |          | GLU | A        | 18  | 6.214  | 21.468 |       | 8.031  | 1.00     | 52.86 |     |    |     | O |
| ATOM   | 28       | CB  |          | GLU | A        | 18  | 4.150  | 23.406 |       | 6.867  | 1.00     | 55.33 |     |    |     | C |
| ATOM   | 29       | CG  |          | GLU | A        | 18  | 3.482  | 24.731 |       | 6.519  | 1.00     | 56.39 |     |    |     | C |
| ATOM   | 30       | CD  |          | GLU | A        | 18  | 2.100  | 24.904 |       | 7.137  | 1.00     | 57.19 |     |    |     | C |
| ATOM   | 31       | OE1 |          | GLU | A        | 18  | 1.559  | 23.935 |       | 7.718  | 1.00     | 56.35 |     |    |     | O |
| ATOM   | 32       | OE2 |          | GLU | A        | 18  | 1.548  | 26.023 |       | 7.028  | 1.00     | 58.12 |     |    |     | O |
| ATOM   | 33       | N   |          | GLU | A        | 19  | 4.526  | 21.260 |       | 9.501  | 1.00     | 51.73 |     |    |     | N |
| ATOM   | 34       | CA  |          | GLU | A        | 19  | 4.823  | 19.867 |       | 9.816  | 1.00     | 50.56 |     |    |     | C |
| ATOM   | 35       | C   |          | GLU | A        | 19  | 4.409  | 18.944 |       | 8.663  | 1.00     | 48.36 |     |    |     | C |
| ATOM   | 36       | O   |          | GLU | A        | 19  | 3.312  | 19.066 |       | 8.102  | 1.00     | 47.54 |     |    |     | O |
| ATOM   | 37       | CB  |          | GLU | A        | 19  | 4.115  | 19.422 |       | 11.100 | 1.00     | 51.05 |     |    |     | C |
| ATOM   | 38       | CG  |          | GLU | A        | 19  | 4.577  | 20.139 |       | 12.360 | 1.00     | 53.53 |     |    |     | C |
| ATOM   | 39       | CD  |          | GLU | A        | 19  | 4.363  | 19.323 |       | 13.638 | 1.00     | 57.67 |     |    |     | C |
| ATOM   | 40       | OE1 |          | GLU | A        | 19  | 3.906  | 18.146 |       | 13.561 | 1.00     | 59.24 |     |    |     | O |
| ATOM   | 41       | OE2 |          | GLU | A        | 19  | 4.663  | 19.864 |       | 14.735 | 1.00     | 59.50 |     |    |     | O |
| ATOM   | 42       | N   |          | ALA | A        | 20  | 5.314  | 18.035 |       | 8.320  | 1.00     | 46.04 |     |    |     | N |
| ATOM   | 43       | CA  |          | ALA | A        | 20  | 5.100  | 17.030 |       | 7.283  | 1.00     | 44.66 |     |    |     | C |
| ATOM   | 44       | C   |          | ALA | A        | 20  | 3.741  | 16.365 |       | 7.394  | 1.00     | 42.92 |     |    |     | C |
| ATOM   | 45       | O   |          | ALA | A        | 20  | 3.230  | 16.154 |       | 8.491  | 1.00     | 42.14 |     |    |     | O |
| ATOM   | 46       | CB  |          | ALA | A        | 20  | 6.182  | 15.965 |       | 7.360  | 1.00     | 44.46 |     |    |     | C |
| ATOM   | 47       | N   |          | GLY | A        | 21  | 3.173  | 16.025 |       | 6.247  | 1.00     | 41.16 |     |    |     | N |
| ATOM   | 48       | CA  |          | GLY | A        | 21  | 1.897  | 15.341 |       | 6.215  | 1.00     | 40.22 |     |    |     | C |
| ATOM   | 49       | C   |          | GLY | A        | 21  | 0.757  | 16.300 |       | 6.480  | 1.00     | 39.27 |     |    |     | C |
| ATOM   | 50       | O   |          | GLY | A        | 21  | -0.309 | 15.895 |       | 6.908  | 1.00     | 38.03 |     |    |     | O |
| ATOM   | 51       | N   |          | ALA | A        | 22  | 1.005  | 17.584 |       | 6.240  | 1.00     | 38.86 |     |    |     | N |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 52  | CA  | ALA | A | 22 | -0.018 | 18.611 | 6.371  | 1.00 | 38.79 | C |
| ATOM | 53  | C   | ALA | A | 22 | -0.618 | 18.613 | 7.758  | 1.00 | 38.64 | C |
| ATOM | 54  | O   | ALA | A | 22 | -1.820 | 18.759 | 7.924  | 1.00 | 38.07 | O |
| ATOM | 55  | CB  | ALA | A | 22 | -1.102 | 18.409 | 5.324  | 1.00 | 38.68 | C |
| ATOM | 56  | N   | LEU | A | 23 | 0.231  | 18.451 | 8.760  | 1.00 | 39.07 | N |
| ATOM | 57  | CA  | LEU | A | 23 | -0.233 | 18.473 | 10.135 | 1.00 | 39.72 | C |
| ATOM | 58  | C   | LEU | A | 23 | -0.290 | 19.886 | 10.692 | 1.00 | 39.39 | C |
| ATOM | 59  | O   | LEU | A | 23 | -0.464 | 20.075 | 11.880 | 1.00 | 39.41 | O |
| ATOM | 60  | CB  | LEU | A | 23 | 0.642  | 17.574 | 11.003 | 1.00 | 40.11 | C |
| ATOM | 61  | CG  | LEU | A | 23 | 0.528  | 16.118 | 10.558 | 1.00 | 41.82 | C |
| ATOM | 62  | CD1 | LEU | A | 23 | 1.414  | 15.185 | 11.384 | 1.00 | 43.18 | C |
| ATOM | 63  | CD2 | LEU | A | 23 | -0.916 | 15.673 | 10.633 | 1.00 | 43.43 | C |
| ATOM | 64  | N   | GLY | A | 24 | -0.156 | 20.879 | 9.823  | 1.00 | 39.21 | N |
| ATOM | 65  | CA  | GLY | A | 24 | -0.290 | 22.258 | 10.237 | 1.00 | 39.16 | C |
| ATOM | 66  | C   | GLY | A | 24 | 0.964  | 22.862 | 10.820 | 1.00 | 39.21 | C |
| ATOM | 67  | O   | GLY | A | 24 | 2.011  | 22.219 | 10.916 | 1.00 | 39.16 | O |
| ATOM | 68  | N   | PRO | A | 25 | 0.854  | 24.118 | 11.223 | 1.00 | 39.08 | N |
| ATOM | 69  | CA  | PRO | A | 25 | 1.997  | 24.830 | 11.775 | 1.00 | 38.84 | C |
| ATOM | 70  | C   | PRO | A | 25 | 2.410  | 24.197 | 13.086 | 1.00 | 38.68 | C |
| ATOM | 71  | O   | PRO | A | 25 | 1.572  | 23.842 | 13.914 | 1.00 | 38.08 | O |
| ATOM | 72  | CB  | PRO | A | 25 | 1.477  | 26.259 | 12.001 | 1.00 | 38.76 | C |
| ATOM | 73  | CG  | PRO | A | 25 | -0.004 | 26.197 | 11.895 | 1.00 | 39.12 | C |
| ATOM | 74  | CD  | PRO | A | 25 | -0.375 | 24.930 | 11.210 | 1.00 | 39.17 | C |
| ATOM | 75  | N   | ALA | A | 26 | 3.713  | 24.037 | 13.246 | 1.00 | 38.92 | N |
| ATOM | 76  | CA  | ALA | A | 26 | 4.269  | 23.489 | 14.467 | 1.00 | 39.38 | C |
| ATOM | 77  | C   | ALA | A | 26 | 3.924  | 24.381 | 15.676 | 1.00 | 38.73 | C |
| ATOM | 78  | O   | ALA | A | 26 | 3.677  | 23.882 | 16.772 | 1.00 | 39.39 | O |
| ATOM | 79  | CB  | ALA | A | 26 | 5.762  | 23.347 | 14.319 | 1.00 | 39.60 | C |
| ATOM | 80  | N   | TRP | A | 27 | 3.871  | 25.687 | 15.468 | 1.00 | 37.43 | N |
| ATOM | 81  | CA  | TRP | A | 27 | 3.516  | 26.602 | 16.543 | 1.00 | 36.82 | C |
| ATOM | 82  | C   | TRP | A | 27 | 3.034  | 27.919 | 15.941 | 1.00 | 36.10 | C |
| ATOM | 83  | O   | TRP | A | 27 | 3.013  | 28.074 | 14.731 | 1.00 | 35.54 | O |
| ATOM | 84  | CB  | TRP | A | 27 | 4.746  | 26.835 | 17.424 | 1.00 | 36.91 | C |
| ATOM | 85  | CG  | TRP | A | 27 | 5.949  | 27.019 | 16.596 | 1.00 | 36.01 | C |
| ATOM | 86  | CD1 | TRP | A | 27 | 6.770  | 26.041 | 16.089 | 1.00 | 36.29 | C |
| ATOM | 87  | CD2 | TRP | A | 27 | 6.450  | 28.249 | 16.107 | 1.00 | 34.41 | C |
| ATOM | 88  | NE1 | TRP | A | 27 | 7.761  | 26.610 | 15.324 | 1.00 | 36.06 | N |
| ATOM | 89  | CE2 | TRP | A | 27 | 7.592  | 27.966 | 15.332 | 1.00 | 34.97 | C |
| ATOM | 90  | CE3 | TRP | A | 27 | 6.066  | 29.568 | 16.263 | 1.00 | 34.24 | C |
| ATOM | 91  | CZ2 | TRP | A | 27 | 8.332  | 28.947 | 14.720 | 1.00 | 36.39 | C |
| ATOM | 92  | CZ3 | TRP | A | 27 | 6.808  | 30.539 | 15.664 | 1.00 | 36.24 | C |
| ATOM | 93  | CH2 | TRP | A | 27 | 7.927  | 30.225 | 14.890 | 1.00 | 36.25 | C |
| ATOM | 94  | N   | ASP | A | 28 | 2.620  | 28.860 | 16.775 | 1.00 | 35.59 | N |
| ATOM | 95  | CA  | ASP | A | 28 | 2.253  | 30.168 | 16.267 | 1.00 | 35.15 | C |
| ATOM | 96  | C   | ASP | A | 28 | 2.816  | 31.224 | 17.160 | 1.00 | 33.93 | C |
| ATOM | 97  | O   | ASP | A | 28 | 3.311  | 30.948 | 18.250 | 1.00 | 33.56 | O |
| ATOM | 98  | CB  | ASP | A | 28 | 0.739  | 30.338 | 16.131 | 1.00 | 36.08 | C |
| ATOM | 99  | CG  | ASP | A | 28 | 0.038  | 30.310 | 17.449 | 1.00 | 38.11 | C |
| ATOM | 100 | OD1 | ASP | A | 28 | -0.096 | 31.392 | 18.076 | 1.00 | 41.06 | O |
| ATOM | 101 | OD2 | ASP | A | 28 | -0.392 | 29.240 | 17.938 | 1.00 | 41.04 | O |
| ATOM | 102 | N   | GLU | A | 29 | 2.737  | 32.448 | 16.665 | 1.00 | 32.84 | N |
| ATOM | 103 | CA  | GLU | A | 29 | 3.288  | 33.615 | 17.330 | 1.00 | 31.31 | C |
| ATOM | 104 | C   | GLU | A | 29 | 2.792  | 33.767 | 18.756 | 1.00 | 29.80 | C |
| ATOM | 105 | O   | GLU | A | 29 | 3.547  | 34.124 | 19.639 | 1.00 | 29.03 | O |
| ATOM | 106 | CB  | GLU | A | 29 | 2.938  | 34.841 | 16.537 | 1.00 | 31.81 | C |
| ATOM | 107 | N   | SER | A | 30 | 1.524  | 33.478 | 18.989 | 1.00 | 28.55 | N |
| ATOM | 108 | CA  | SER | A | 30 | 0.957  | 33.680 | 20.314 | 1.00 | 28.00 | C |
| ATOM | 109 | C   | SER | A | 30 | 1.613  | 32.830 | 21.391 | 1.00 | 27.25 | C |
| ATOM | 110 | O   | SER | A | 30 | 1.360  | 33.035 | 22.563 | 1.00 | 26.88 | O |
| ATOM | 111 | CB  | SER | A | 30 | -0.546 | 33.404 | 20.302 | 1.00 | 27.71 | C |
| ATOM | 112 | OG  | SER | A | 30 | -0.800 | 32.015 | 20.328 | 1.00 | 28.97 | O |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 113 | N   | GLN | A | 31 | 2.434  | 31.864 | 20.994 | 1.00 | 26.92 | N |
| ATOM | 114 | CA  | GLN | A | 31 | 3.089  | 30.988 | 21.950 | 1.00 | 26.85 | C |
| ATOM | 115 | C   | GLN | A | 31 | 4.447  | 31.558 | 22.362 | 1.00 | 26.63 | C |
| ATOM | 116 | O   | GLN | A | 31 | 5.115  | 30.995 | 23.220 | 1.00 | 25.89 | O |
| ATOM | 117 | CB  | GLN | A | 31 | 3.270  | 29.576 | 21.375 | 1.00 | 26.90 | C |
| ATOM | 118 | CG  | GLN | A | 31 | 1.975  | 28.816 | 21.097 | 1.00 | 27.50 | C |
| ATOM | 119 | CD  | GLN | A | 31 | 2.227  | 27.446 | 20.480 | 1.00 | 27.30 | C |
| ATOM | 120 | OE1 | GLN | A | 31 | 2.332  | 27.330 | 19.262 | 1.00 | 28.39 | O |
| ATOM | 121 | NE2 | GLN | A | 31 | 2.354  | 26.419 | 21.319 | 1.00 | 23.43 | N |
| ATOM | 122 | N   | LEU | A | 32 | 4.835  | 32.682 | 21.757 | 1.00 | 26.56 | N |
| ATOM | 123 | CA  | LEU | A | 32 | 6.094  | 33.351 | 22.078 | 1.00 | 26.88 | C |
| ATOM | 124 | C   | LEU | A | 32 | 5.854  | 34.500 | 23.047 | 1.00 | 26.64 | C |
| ATOM | 125 | O   | LEU | A | 32 | 4.875  | 35.214 | 22.913 | 1.00 | 26.22 | O |
| ATOM | 126 | CB  | LEU | A | 32 | 6.743  | 33.906 | 20.807 | 1.00 | 26.71 | C |
| ATOM | 127 | CG  | LEU | A | 32 | 7.054  | 32.866 | 19.724 | 1.00 | 29.00 | C |
| ATOM | 128 | CD1 | LEU | A | 32 | 7.704  | 33.537 | 18.535 | 1.00 | 31.11 | C |
| ATOM | 129 | CD2 | LEU | A | 32 | 7.942  | 31.773 | 20.245 | 1.00 | 28.07 | C |
| ATOM | 130 | N   | ARG | A | 33 | 6.737  | 34.671 | 24.026 | 1.00 | 26.49 | N |
| ATOM | 131 | CA  | ARG | A | 33 | 6.622  | 35.799 | 24.957 | 1.00 | 26.48 | C |
| ATOM | 132 | C   | ARG | A | 33 | 7.070  | 37.071 | 24.252 | 1.00 | 26.68 | C |
| ATOM | 133 | O   | ARG | A | 33 | 7.810  | 37.025 | 23.280 | 1.00 | 26.97 | O |
| ATOM | 134 | CB  | ARG | A | 33 | 7.454  | 35.554 | 26.224 | 1.00 | 26.44 | C |
| ATOM | 135 | CG  | ARG | A | 33 | 7.071  | 34.261 | 26.976 | 1.00 | 25.53 | C |
| ATOM | 136 | CD  | ARG | A | 33 | 7.869  | 34.029 | 28.245 | 1.00 | 25.76 | C |
| ATOM | 137 | NE  | ARG | A | 33 | 7.329  | 32.926 | 29.021 | 1.00 | 25.87 | N |
| ATOM | 138 | CZ  | ARG | A | 33 | 6.418  | 33.033 | 29.969 | 1.00 | 25.35 | C |
| ATOM | 139 | NH1 | ARG | A | 33 | 5.916  | 34.198 | 30.309 | 1.00 | 24.02 | N |
| ATOM | 140 | NH2 | ARG | A | 33 | 6.003  | 31.941 | 30.587 | 1.00 | 28.18 | N |
| ATOM | 141 | N   | SER | A | 34 | 6.643  | 38.214 | 24.751 | 1.00 | 26.73 | N |
| ATOM | 142 | CA  | SER | A | 34 | 6.939  | 39.469 | 24.090 | 1.00 | 27.21 | C |
| ATOM | 143 | C   | SER | A | 34 | 8.021  | 40.251 | 24.840 | 1.00 | 26.40 | C |
| ATOM | 144 | O   | SER | A | 34 | 7.957  | 40.391 | 26.046 | 1.00 | 25.65 | O |
| ATOM | 145 | CB  | SER | A | 34 | 5.657  | 40.278 | 24.028 | 1.00 | 27.92 | C |
| ATOM | 146 | OG  | SER | A | 34 | 5.402  | 40.780 | 25.323 | 1.00 | 31.78 | O |
| ATOM | 147 | N   | TYR | A | 35 | 9.009  | 40.750 | 24.110 | 1.00 | 26.09 | N |
| ATOM | 148 | CA  | TYR | A | 35 | 10.169 | 41.390 | 24.711 | 1.00 | 26.44 | C |
| ATOM | 149 | C   | TYR | A | 35 | 10.412 | 42.731 | 24.046 | 1.00 | 27.00 | C |
| ATOM | 150 | O   | TYR | A | 35 | 9.815  | 43.009 | 23.028 | 1.00 | 27.14 | O |
| ATOM | 151 | CB  | TYR | A | 35 | 11.386 | 40.479 | 24.577 | 1.00 | 25.83 | C |
| ATOM | 152 | CG  | TYR | A | 35 | 11.217 | 39.198 | 25.357 | 1.00 | 25.49 | C |
| ATOM | 153 | CD1 | TYR | A | 35 | 11.041 | 39.226 | 26.739 | 1.00 | 23.65 | C |
| ATOM | 154 | CD2 | TYR | A | 35 | 11.219 | 37.963 | 24.723 | 1.00 | 23.87 | C |
| ATOM | 155 | CE1 | TYR | A | 35 | 10.869 | 38.063 | 27.459 | 1.00 | 23.41 | C |
| ATOM | 156 | CE2 | TYR | A | 35 | 11.061 | 36.795 | 25.445 | 1.00 | 24.37 | C |
| ATOM | 157 | CZ  | TYR | A | 35 | 10.881 | 36.847 | 26.809 | 1.00 | 22.92 | C |
| ATOM | 158 | OH  | TYR | A | 35 | 10.698 | 35.686 | 27.522 | 1.00 | 23.94 | O |
| ATOM | 159 | N   | SER | A | 36 | 11.326 | 43.531 | 24.596 | 1.00 | 27.45 | N |
| ATOM | 160 | CA  | SER | A | 36 | 11.555 | 44.905 | 24.127 | 1.00 | 27.58 | C |
| ATOM | 161 | C   | SER | A | 36 | 12.553 | 45.092 | 22.987 | 1.00 | 27.13 | C |
| ATOM | 162 | O   | SER | A | 36 | 12.764 | 46.211 | 22.533 | 1.00 | 27.71 | O |
| ATOM | 163 | CB  | SER | A | 36 | 12.109 | 45.724 | 25.286 | 1.00 | 27.62 | C |
| ATOM | 164 | OG  | SER | A | 36 | 13.365 | 45.201 | 25.697 | 1.00 | 27.53 | O |
| ATOM | 165 | N   | PHE | A | 37 | 13.181 | 44.025 | 22.543 | 1.00 | 25.62 | N |
| ATOM | 166 | CA  | PHE | A | 37 | 14.263 | 44.169 | 21.590 | 1.00 | 24.95 | C |
| ATOM | 167 | C   | PHE | A | 37 | 13.949 | 43.447 | 20.301 | 1.00 | 25.32 | C |
| ATOM | 168 | O   | PHE | A | 37 | 13.191 | 42.512 | 20.274 | 1.00 | 25.29 | O |
| ATOM | 169 | CB  | PHE | A | 37 | 15.537 | 43.571 | 22.185 | 1.00 | 23.88 | C |
| ATOM | 170 | CG  | PHE | A | 37 | 15.340 | 42.162 | 22.731 | 1.00 | 22.69 | C |
| ATOM | 171 | CD1 | PHE | A | 37 | 15.353 | 41.077 | 21.890 | 1.00 | 20.43 | C |
| ATOM | 172 | CD2 | PHE | A | 37 | 15.104 | 41.949 | 24.076 | 1.00 | 23.12 | C |
| ATOM | 173 | CE1 | PHE | A | 37 | 15.160 | 39.778 | 22.386 | 1.00 | 22.83 | C |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 174 | CE2 | PHE | A | 37 | 14.920 | 40.666 | 24.578 | 1.00 | 22.73 | C |
| ATOM | 175 | CZ  | PHE | A | 37 | 14.944 | 39.585 | 23.737 | 1.00 | 22.04 | C |
| ATOM | 176 | N   | PRO | A | 38 | 14.533 | 43.907 | 19.222 | 1.00 | 25.57 | N |
| ATOM | 177 | CA  | PRO | A | 38 | 14.396 | 43.216 | 17.950 | 1.00 | 25.50 | C |
| ATOM | 178 | C   | PRO | A | 38 | 15.321 | 42.002 | 17.861 | 1.00 | 25.35 | C |
| ATOM | 179 | O   | PRO | A | 38 | 16.280 | 41.887 | 18.640 | 1.00 | 25.01 | O |
| ATOM | 180 | CB  | PRO | A | 38 | 14.815 | 44.278 | 16.944 | 1.00 | 25.31 | C |
| ATOM | 181 | CG  | PRO | A | 38 | 15.776 | 45.181 | 17.729 | 1.00 | 26.61 | C |
| ATOM | 182 | CD  | PRO | A | 38 | 15.271 | 45.178 | 19.125 | 1.00 | 25.73 | C |
| ATOM | 183 | N   | THR | A | 39 | 15.032 | 41.124 | 16.902 | 1.00 | 24.60 | N |
| ATOM | 184 | CA  | THR | A | 39 | 15.876 | 39.979 | 16.607 | 1.00 | 24.58 | C |
| ATOM | 185 | C   | THR | A | 39 | 15.881 | 39.686 | 15.112 | 1.00 | 25.39 | C |
| ATOM | 186 | O   | THR | A | 39 | 15.004 | 40.121 | 14.383 | 1.00 | 24.72 | O |
| ATOM | 187 | CB  | THR | A | 39 | 15.364 | 38.721 | 17.295 | 1.00 | 24.33 | C |
| ATOM | 188 | OG1 | THR | A | 39 | 14.023 | 38.453 | 16.860 | 1.00 | 21.36 | O |
| ATOM | 189 | CG2 | THR | A | 39 | 15.256 | 38.892 | 18.832 | 1.00 | 23.91 | C |
| ATOM | 190 | N   | ARG | A | 40 | 16.875 | 38.912 | 14.692 | 1.00 | 26.09 | N |
| ATOM | 191 | CA  | ARG | A | 40 | 17.000 | 38.399 | 13.337 | 1.00 | 26.92 | C |
| ATOM | 192 | C   | ARG | A | 40 | 17.057 | 36.884 | 13.469 | 1.00 | 26.73 | C |
| ATOM | 193 | O   | ARG | A | 40 | 17.407 | 36.366 | 14.517 | 1.00 | 26.53 | O |
| ATOM | 194 | CB  | ARG | A | 40 | 18.291 | 38.888 | 12.696 | 1.00 | 27.12 | C |
| ATOM | 195 | CG  | ARG | A | 40 | 18.289 | 40.360 | 12.400 | 1.00 | 32.37 | C |
| ATOM | 196 | CD  | ARG | A | 40 | 16.925 | 40.858 | 11.994 | 1.00 | 36.79 | C |
| ATOM | 197 | NE  | ARG | A | 40 | 16.783 | 41.137 | 10.583 | 1.00 | 41.20 | N |
| ATOM | 198 | CZ  | ARG | A | 40 | 15.617 | 41.408 | 10.023 | 1.00 | 46.28 | C |
| ATOM | 199 | NH1 | ARG | A | 40 | 14.512 | 41.388 | 10.768 | 1.00 | 47.83 | N |
| ATOM | 200 | NH2 | ARG | A | 40 | 15.548 | 41.708 | 8.731  | 1.00 | 48.02 | N |
| ATOM | 201 | N   | PRO | A | 41 | 16.728 | 36.163 | 12.413 | 1.00 | 26.96 | N |
| ATOM | 202 | CA  | PRO | A | 41 | 16.709 | 34.706 | 12.510 | 1.00 | 27.17 | C |
| ATOM | 203 | C   | PRO | A | 41 | 18.085 | 34.054 | 12.469 | 1.00 | 26.50 | C |
| ATOM | 204 | O   | PRO | A | 41 | 19.002 | 34.538 | 11.830 | 1.00 | 26.34 | O |
| ATOM | 205 | CB  | PRO | A | 41 | 15.867 | 34.277 | 11.298 | 1.00 | 27.12 | C |
| ATOM | 206 | CG  | PRO | A | 41 | 16.027 | 35.434 | 10.296 | 1.00 | 27.66 | C |
| ATOM | 207 | CD  | PRO | A | 41 | 16.337 | 36.661 | 11.077 | 1.00 | 26.70 | C |
| ATOM | 208 | N   | ILE | A | 42 | 18.214 | 32.951 | 13.185 | 1.00 | 25.35 | N |
| ATOM | 209 | CA  | ILE | A | 42 | 19.400 | 32.143 | 13.070 | 1.00 | 24.29 | C |
| ATOM | 210 | C   | ILE | A | 42 | 19.161 | 31.290 | 11.832 | 1.00 | 23.98 | C |
| ATOM | 211 | O   | ILE | A | 42 | 18.050 | 30.793 | 11.632 | 1.00 | 24.20 | O |
| ATOM | 212 | CB  | ILE | A | 42 | 19.530 | 31.283 | 14.302 | 1.00 | 24.58 | C |
| ATOM | 213 | CG1 | ILE | A | 42 | 19.779 | 32.181 | 15.518 | 1.00 | 22.71 | C |
| ATOM | 214 | CG2 | ILE | A | 42 | 20.644 | 30.233 | 14.113 | 1.00 | 24.95 | C |
| ATOM | 215 | CD1 | ILE | A | 42 | 19.466 | 31.516 | 16.837 | 1.00 | 22.70 | C |
| ATOM | 216 | N   | PRO | A | 43 | 20.168 | 31.122 | 10.989 | 1.00 | 23.44 | N |
| ATOM | 217 | CA  | PRO | A | 43 | 20.016 | 30.276 | 9.807  | 1.00 | 23.74 | C |
| ATOM | 218 | C   | PRO | A | 43 | 19.709 | 28.802 | 10.154 | 1.00 | 24.82 | C |
| ATOM | 219 | O   | PRO | A | 43 | 20.281 | 28.292 | 11.130 | 1.00 | 24.03 | O |
| ATOM | 220 | CB  | PRO | A | 43 | 21.372 | 30.397 | 9.107  | 1.00 | 24.23 | C |
| ATOM | 221 | CG  | PRO | A | 43 | 22.071 | 31.602 | 9.740  | 1.00 | 23.91 | C |
| ATOM | 222 | CD  | PRO | A | 43 | 21.504 | 31.737 | 11.092 | 1.00 | 23.12 | C |
| ATOM | 223 | N   | ARG | A | 44 | 18.784 | 28.178 | 9.406  | 1.00 | 25.20 | N |
| ATOM | 224 | CA  | ARG | A | 44 | 18.439 | 26.767 | 9.520  | 1.00 | 26.19 | C |
| ATOM | 225 | C   | ARG | A | 44 | 18.977 | 26.125 | 8.269  | 1.00 | 25.69 | C |
| ATOM | 226 | O   | ARG | A | 44 | 18.563 | 26.468 | 7.159  | 1.00 | 25.67 | O |
| ATOM | 227 | CB  | ARG | A | 44 | 16.934 | 26.504 | 9.513  | 1.00 | 27.16 | C |
| ATOM | 228 | CG  | ARG | A | 44 | 16.140 | 27.062 | 10.678 | 1.00 | 31.24 | C |
| ATOM | 229 | CD  | ARG | A | 44 | 14.653 | 26.529 | 10.769 | 1.00 | 32.98 | C |
| ATOM | 230 | NE  | ARG | A | 44 | 14.400 | 25.143 | 10.311 | 1.00 | 34.09 | N |
| ATOM | 231 | CZ  | ARG | A | 44 | 14.258 | 24.070 | 11.128 | 1.00 | 33.28 | C |
| ATOM | 232 | NH1 | ARG | A | 44 | 14.384 | 24.177 | 12.453 | 1.00 | 29.63 | N |
| ATOM | 233 | NH2 | ARG | A | 44 | 13.995 | 22.873 | 10.617 | 1.00 | 34.28 | N |
| ATOM | 234 | N   | LEU | A | 45 | 19.870 | 25.174 | 8.433  | 1.00 | 24.68 | N |



|      |     |     |     |   |    |        |        |       |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|-------|------|-------|---|
| ATOM | 235 | CA  | LEU | A | 45 | 20.551 | 24.608 | 7.302 | 1.00 | 24.30 | C |
| ATOM | 236 | C   | LEU | A | 45 | 20.768 | 23.134 | 7.471 | 1.00 | 24.39 | C |
| ATOM | 237 | O   | LEU | A | 45 | 20.711 | 22.623 | 8.588 | 1.00 | 23.97 | O |
| ATOM | 238 | CB  | LEU | A | 45 | 21.934 | 25.233 | 7.205 | 1.00 | 23.42 | C |
| ATOM | 239 | CG  | LEU | A | 45 | 21.929 | 26.724 | 6.941 | 1.00 | 24.95 | C |
| ATOM | 240 | CD1 | LEU | A | 45 | 23.339 | 27.284 | 7.080 | 1.00 | 26.26 | C |
| ATOM | 241 | CD2 | LEU | A | 45 | 21.375 | 26.953 | 5.533 | 1.00 | 24.54 | C |
| ATOM | 242 | N   | SER | A | 46 | 21.092 | 22.494 | 6.352 | 1.00 | 24.71 | N |
| ATOM | 243 | CA  | SER | A | 46 | 21.498 | 21.119 | 6.345 | 1.00 | 25.24 | C |
| ATOM | 244 | C   | SER | A | 46 | 22.930 | 21.043 | 6.804 | 1.00 | 25.58 | C |
| ATOM | 245 | O   | SER | A | 46 | 23.741 | 21.908 | 6.522 | 1.00 | 24.65 | O |
| ATOM | 246 | CB  | SER | A | 46 | 21.401 | 20.505 | 4.950 | 1.00 | 25.11 | C |
| ATOM | 247 | OG  | SER | A | 46 | 21.863 | 19.150 | 4.965 | 1.00 | 24.50 | O |
| ATOM | 248 | N   | GLN | A | 47 | 23.208 | 19.970 | 7.517 | 1.00 | 26.68 | N |
| ATOM | 249 | CA  | GLN | A | 47 | 24.524 | 19.626 | 8.011 | 1.00 | 27.63 | C |
| ATOM | 250 | C   | GLN | A | 47 | 25.510 | 19.442 | 6.853 | 1.00 | 28.01 | C |
| ATOM | 251 | O   | GLN | A | 47 | 26.704 | 19.613 | 7.026 | 1.00 | 28.15 | O |
| ATOM | 252 | CB  | GLN | A | 47 | 24.368 | 18.317 | 8.803 | 1.00 | 28.89 | C |
| ATOM | 253 | CG  | GLN | A | 47 | 25.580 | 17.447 | 8.920 | 1.00 | 31.28 | C |
| ATOM | 254 | CD  | GLN | A | 47 | 25.826 | 16.556 | 7.765 | 1.00 | 32.33 | C |
| ATOM | 255 | OE1 | GLN | A | 47 | 24.906 | 16.149 | 7.048 | 1.00 | 37.08 | O |
| ATOM | 256 | NE2 | GLN | A | 47 | 27.089 | 16.213 | 7.576 | 1.00 | 35.81 | N |
| ATOM | 257 | N   | SER | A | 48 | 25.026 | 19.086 | 5.667 | 1.00 | 28.11 | N |
| ATOM | 258 | CA  | SER | A | 48 | 25.930 | 18.925 | 4.524 | 1.00 | 28.72 | C |
| ATOM | 259 | C   | SER | A | 48 | 26.222 | 20.262 | 3.828 | 1.00 | 29.21 | C |
| ATOM | 260 | O   | SER | A | 48 | 27.068 | 20.339 | 2.936 | 1.00 | 29.21 | O |
| ATOM | 261 | CB  | SER | A | 48 | 25.343 | 17.952 | 3.508 | 1.00 | 28.66 | C |
| ATOM | 262 | OG  | SER | A | 48 | 24.111 | 18.440 | 2.993 | 1.00 | 29.43 | O |
| ATOM | 263 | N   | ASP | A | 49 | 25.525 | 21.314 | 4.236 | 1.00 | 29.60 | N |
| ATOM | 264 | CA  | ASP | A | 49 | 25.683 | 22.610 | 3.596 | 1.00 | 30.12 | C |
| ATOM | 265 | C   | ASP | A | 49 | 26.949 | 23.307 | 4.087 | 1.00 | 30.43 | C |
| ATOM | 266 | O   | ASP | A | 49 | 27.100 | 23.565 | 5.272 | 1.00 | 29.60 | O |
| ATOM | 267 | CB  | ASP | A | 49 | 24.450 | 23.458 | 3.858 | 1.00 | 30.26 | C |
| ATOM | 268 | CG  | ASP | A | 49 | 24.491 | 24.792 | 3.151 | 1.00 | 31.74 | C |
| ATOM | 269 | OD1 | ASP | A | 49 | 25.589 | 25.306 | 2.859 | 1.00 | 31.79 | O |
| ATOM | 270 | OD2 | ASP | A | 49 | 23.454 | 25.418 | 2.878 | 1.00 | 34.13 | O |
| ATOM | 271 | N   | PRO | A | 50 | 27.829 | 23.668 | 3.155 | 1.00 | 31.31 | N |
| ATOM | 272 | CA  | PRO | A | 50 | 29.123 | 24.273 | 3.499 | 1.00 | 31.63 | C |
| ATOM | 273 | C   | PRO | A | 50 | 28.965 | 25.514 | 4.355 | 1.00 | 31.72 | C |
| ATOM | 274 | O   | PRO | A | 50 | 29.849 | 25.807 | 5.164 | 1.00 | 31.85 | O |
| ATOM | 275 | CB  | PRO | A | 50 | 29.726 | 24.643 | 2.124 | 1.00 | 31.53 | C |
| ATOM | 276 | CG  | PRO | A | 50 | 29.036 | 23.738 | 1.168 | 1.00 | 32.13 | C |
| ATOM | 277 | CD  | PRO | A | 50 | 27.624 | 23.620 | 1.697 | 1.00 | 31.55 | C |
| ATOM | 278 | N   | ARG | A | 51 | 27.875 | 26.246 | 4.171 | 1.00 | 32.04 | N |
| ATOM | 279 | CA  | ARG | A | 51 | 27.648 | 27.443 | 4.962 | 1.00 | 32.56 | C |
| ATOM | 280 | C   | ARG | A | 51 | 27.478 | 27.078 | 6.439 | 1.00 | 32.09 | C |
| ATOM | 281 | O   | ARG | A | 51 | 27.853 | 27.855 | 7.322 | 1.00 | 31.87 | O |
| ATOM | 282 | CB  | ARG | A | 51 | 26.420 | 28.221 | 4.464 | 1.00 | 32.95 | C |
| ATOM | 283 | CG  | ARG | A | 51 | 26.568 | 28.810 | 3.064 | 1.00 | 34.79 | C |
| ATOM | 284 | CD  | ARG | A | 51 | 25.273 | 29.372 | 2.480 | 1.00 | 35.89 | C |
| ATOM | 285 | NE  | ARG | A | 51 | 24.276 | 28.325 | 2.228 | 1.00 | 37.56 | N |
| ATOM | 286 | CZ  | ARG | A | 51 | 22.982 | 28.564 | 2.061 | 1.00 | 39.54 | C |
| ATOM | 287 | NH1 | ARG | A | 51 | 22.531 | 29.814 | 2.124 | 1.00 | 40.85 | N |
| ATOM | 288 | NH2 | ARG | A | 51 | 22.135 | 27.573 | 1.823 | 1.00 | 38.55 | N |
| ATOM | 289 | N   | ALA | A | 52 | 26.932 | 25.903 | 6.721 | 1.00 | 31.50 | N |
| ATOM | 290 | CA  | ALA | A | 52 | 26.769 | 25.513 | 8.117 | 1.00 | 31.34 | C |
| ATOM | 291 | C   | ALA | A | 52 | 28.135 | 25.310 | 8.744 | 1.00 | 31.24 | C |
| ATOM | 292 | O   | ALA | A | 52 | 28.409 | 25.763 | 9.865 | 1.00 | 30.91 | O |
| ATOM | 293 | CB  | ALA | A | 52 | 25.953 | 24.284 | 8.236 | 1.00 | 31.35 | C |
| ATOM | 294 | N   | GLU | A | 53 | 29.005 | 24.652 | 8.005 | 1.00 | 30.92 | N |
| ATOM | 295 | CA  | GLU | A | 53 | 30.332 | 24.404 | 8.501 | 1.00 | 31.92 | C |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 296 | C   | GLU | A | 53 | 31.059 | 25.730 | 8.728  | 1.00 | 31.52 | C |
| ATOM | 297 | O   | GLU | A | 53 | 31.766 | 25.898 | 9.717  | 1.00 | 30.52 | O |
| ATOM | 298 | CB  | GLU | A | 53 | 31.119 | 23.554 | 7.525  | 1.00 | 32.10 | C |
| ATOM | 299 | CG  | GLU | A | 53 | 32.216 | 22.795 | 8.229  | 1.00 | 36.08 | C |
| ATOM | 300 | CD  | GLU | A | 53 | 31.776 | 21.411 | 8.717  | 1.00 | 39.44 | C |
| ATOM | 301 | OE1 | GLU | A | 53 | 30.629 | 21.234 | 9.167  | 1.00 | 40.34 | O |
| ATOM | 302 | OE2 | GLU | A | 53 | 32.606 | 20.487 | 8.652  | 1.00 | 43.45 | O |
| ATOM | 303 | N   | GLU | A | 54 | 30.870 | 26.665 | 7.808  | 1.00 | 31.32 | N |
| ATOM | 304 | CA  | GLU | A | 54 | 31.507 | 27.968 | 7.919  | 1.00 | 32.09 | C |
| ATOM | 305 | C   | GLU | A | 54 | 31.039 | 28.685 | 9.193  | 1.00 | 31.07 | C |
| ATOM | 306 | O   | GLU | A | 54 | 31.833 | 29.295 | 9.881  | 1.00 | 31.27 | O |
| ATOM | 307 | CB  | GLU | A | 54 | 31.218 | 28.812 | 6.681  | 1.00 | 32.42 | C |
| ATOM | 308 | CG  | GLU | A | 54 | 31.939 | 30.146 | 6.669  | 1.00 | 37.01 | C |
| ATOM | 309 | CD  | GLU | A | 54 | 31.662 | 30.966 | 5.410  | 1.00 | 40.45 | C |
| ATOM | 310 | OE1 | GLU | A | 54 | 30.843 | 30.528 | 4.558  | 1.00 | 41.94 | O |
| ATOM | 311 | OE2 | GLU | A | 54 | 32.268 | 32.051 | 5.285  | 1.00 | 43.43 | O |
| ATOM | 312 | N   | LEU | A | 55 | 29.761 | 28.567 | 9.534  | 1.00 | 29.85 | N |
| ATOM | 313 | CA  | LEU | A | 55 | 29.251 | 29.240 | 10.708 | 1.00 | 28.58 | C |
| ATOM | 314 | C   | LEU | A | 55 | 29.848 | 28.667 | 11.983 | 1.00 | 27.91 | C |
| ATOM | 315 | O   | LEU | A | 55 | 30.304 | 29.419 | 12.841 | 1.00 | 26.43 | O |
| ATOM | 316 | CB  | LEU | A | 55 | 27.734 | 29.179 | 10.733 | 1.00 | 28.61 | C |
| ATOM | 317 | CG  | LEU | A | 55 | 27.097 | 30.041 | 9.652  | 1.00 | 28.69 | C |
| ATOM | 318 | CD1 | LEU | A | 55 | 25.647 | 29.633 | 9.423  | 1.00 | 29.69 | C |
| ATOM | 319 | CD2 | LEU | A | 55 | 27.193 | 31.507 | 10.005 | 1.00 | 27.60 | C |
| ATOM | 320 | N   | ILE | A | 56 | 29.889 | 27.334 | 12.086 | 1.00 | 27.51 | N |
| ATOM | 321 | CA  | ILE | A | 56 | 30.432 | 26.679 | 13.278 | 1.00 | 27.49 | C |
| ATOM | 322 | C   | ILE | A | 56 | 31.910 | 27.014 | 13.457 | 1.00 | 28.32 | C |
| ATOM | 323 | O   | ILE | A | 56 | 32.359 | 27.353 | 14.549 | 1.00 | 28.51 | O |
| ATOM | 324 | CB  | ILE | A | 56 | 30.260 | 25.174 | 13.192 | 1.00 | 27.21 | C |
| ATOM | 325 | CG1 | ILE | A | 56 | 28.771 | 24.787 | 13.218 | 1.00 | 25.69 | C |
| ATOM | 326 | CG2 | ILE | A | 56 | 30.982 | 24.505 | 14.354 | 1.00 | 27.65 | C |
| ATOM | 327 | CD1 | ILE | A | 56 | 28.484 | 23.341 | 12.760 | 1.00 | 23.98 | C |
| ATOM | 328 | N   | GLU | A | 57 | 32.645 | 26.935 | 12.357 | 1.00 | 28.85 | N |
| ATOM | 329 | CA  | GLU | A | 57 | 34.068 | 27.230 | 12.308 | 1.00 | 29.98 | C |
| ATOM | 330 | C   | GLU | A | 57 | 34.319 | 28.623 | 12.837 | 1.00 | 30.12 | C |
| ATOM | 331 | O   | GLU | A | 57 | 35.306 | 28.869 | 13.524 | 1.00 | 31.00 | O |
| ATOM | 332 | CB  | GLU | A | 57 | 34.557 | 27.137 | 10.850 | 1.00 | 30.52 | C |
| ATOM | 333 | CG  | GLU | A | 57 | 36.003 | 27.518 | 10.610 | 1.00 | 33.37 | C |
| ATOM | 334 | CD  | GLU | A | 57 | 36.968 | 26.742 | 11.482 | 1.00 | 38.19 | C |
| ATOM | 335 | OE1 | GLU | A | 57 | 36.689 | 25.558 | 11.810 | 1.00 | 41.02 | O |
| ATOM | 336 | OE2 | GLU | A | 57 | 38.015 | 27.329 | 11.847 | 1.00 | 42.74 | O |
| ATOM | 337 | N   | ASN | A | 58 | 33.409 | 29.527 | 12.516 | 1.00 | 29.57 | N |
| ATOM | 338 | CA  | ASN | A | 58 | 33.516 | 30.911 | 12.929 | 1.00 | 29.62 | C |
| ATOM | 339 | C   | ASN | A | 58 | 32.852 | 31.222 | 14.230 | 1.00 | 27.88 | C |
| ATOM | 340 | O   | ASN | A | 58 | 32.690 | 32.364 | 14.566 | 1.00 | 26.74 | O |
| ATOM | 341 | CB  | ASN | A | 58 | 32.805 | 31.769 | 11.918 | 1.00 | 30.43 | C |
| ATOM | 342 | CG  | ASN | A | 58 | 33.719 | 32.439 | 11.040 | 1.00 | 33.87 | C |
| ATOM | 343 | OD1 | ASN | A | 58 | 34.040 | 31.918 | 9.965  | 1.00 | 36.67 | O |
| ATOM | 344 | ND2 | ASN | A | 58 | 34.189 | 33.629 | 11.467 | 1.00 | 38.66 | N |
| ATOM | 345 | N   | GLU | A | 59 | 32.396 | 30.205 | 14.922 | 1.00 | 27.73 | N |
| ATOM | 346 | CA  | GLU | A | 59 | 31.753 | 30.411 | 16.205 | 1.00 | 27.50 | C |
| ATOM | 347 | C   | GLU | A | 59 | 30.545 | 31.320 | 16.104 | 1.00 | 26.07 | C |
| ATOM | 348 | O   | GLU | A | 59 | 30.366 | 32.255 | 16.861 | 1.00 | 25.28 | O |
| ATOM | 349 | CB  | GLU | A | 59 | 32.795 | 30.867 | 17.224 | 1.00 | 28.12 | C |
| ATOM | 350 | CG  | GLU | A | 59 | 33.720 | 29.688 | 17.531 | 1.00 | 31.06 | C |
| ATOM | 351 | CD  | GLU | A | 59 | 34.739 | 29.965 | 18.604 | 1.00 | 35.24 | C |
| ATOM | 352 | OE1 | GLU | A | 59 | 35.826 | 30.432 | 18.239 | 1.00 | 39.24 | O |
| ATOM | 353 | OE2 | GLU | A | 59 | 34.469 | 29.698 | 19.795 | 1.00 | 37.54 | O |
| ATOM | 354 | N   | GLU | A | 60 | 29.691 | 30.982 | 15.155 | 1.00 | 25.70 | N |
| ATOM | 355 | CA  | GLU | A | 60 | 28.417 | 31.643 | 14.971 | 1.00 | 25.50 | C |
| ATOM | 356 | C   | GLU | A | 60 | 27.345 | 30.576 | 14.998 | 1.00 | 24.10 | C |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 357 | O   | GLU | A | 60 | 27.527 | 29.479 | 14.487 | 1.00 | 22.92 | O |
| ATOM | 358 | CB  | GLU | A | 60 | 28.402 | 32.404 | 13.664 | 1.00 | 25.96 | C |
| ATOM | 359 | CG  | GLU | A | 60 | 29.454 | 33.497 | 13.697 | 1.00 | 30.39 | C |
| ATOM | 360 | CD  | GLU | A | 60 | 29.218 | 34.599 | 12.703 | 1.00 | 35.90 | C |
| ATOM | 361 | OE1 | GLU | A | 60 | 29.281 | 34.349 | 11.478 | 1.00 | 38.45 | O |
| ATOM | 362 | OE2 | GLU | A | 60 | 28.998 | 35.732 | 13.165 | 1.00 | 43.84 | O |
| ATOM | 363 | N   | PRO | A | 61 | 26.203 | 30.933 | 15.546 | 1.00 | 22.92 | N |
| ATOM | 364 | CA  | PRO | A | 61 | 25.112 | 29.983 | 15.735 | 1.00 | 22.31 | C |
| ATOM | 365 | C   | PRO | A | 61 | 24.482 | 29.519 | 14.445 | 1.00 | 21.76 | C |
| ATOM | 366 | O   | PRO | A | 61 | 24.394 | 30.252 | 13.474 | 1.00 | 21.59 | O |
| ATOM | 367 | CB  | PRO | A | 61 | 24.079 | 30.775 | 16.525 | 1.00 | 22.55 | C |
| ATOM | 368 | CG  | PRO | A | 61 | 24.450 | 32.218 | 16.380 | 1.00 | 21.42 | C |
| ATOM | 369 | CD  | PRO | A | 61 | 25.863 | 32.295 | 15.967 | 1.00 | 22.38 | C |
| ATOM | 370 | N   | VAL | A | 62 | 24.032 | 28.279 | 14.444 | 1.00 | 21.55 | N |
| ATOM | 371 | CA  | VAL | A | 62 | 23.306 | 27.739 | 13.317 | 1.00 | 21.90 | C |
| ATOM | 372 | C   | VAL | A | 62 | 22.415 | 26.622 | 13.817 | 1.00 | 22.38 | C |
| ATOM | 373 | O   | VAL | A | 62 | 22.771 | 25.886 | 14.757 | 1.00 | 22.77 | O |
| ATOM | 374 | CB  | VAL | A | 62 | 24.262 | 27.217 | 12.218 | 1.00 | 22.10 | C |
| ATOM | 375 | CG1 | VAL | A | 62 | 25.134 | 26.112 | 12.738 | 1.00 | 22.89 | C |
| ATOM | 376 | CG2 | VAL | A | 62 | 23.486 | 26.748 | 11.000 | 1.00 | 21.98 | C |
| ATOM | 377 | N   | VAL | A | 63 | 21.234 | 26.517 | 13.226 | 1.00 | 22.90 | N |
| ATOM | 378 | CA  | VAL | A | 63 | 20.373 | 25.398 | 13.499 | 1.00 | 23.20 | C |
| ATOM | 379 | C   | VAL | A | 63 | 20.586 | 24.373 | 12.378 | 1.00 | 23.18 | C |
| ATOM | 380 | O   | VAL | A | 63 | 20.395 | 24.682 | 11.208 | 1.00 | 23.38 | O |
| ATOM | 381 | CB  | VAL | A | 63 | 18.880 | 25.768 | 13.561 | 1.00 | 23.27 | C |
| ATOM | 382 | CG1 | VAL | A | 63 | 18.046 | 24.483 | 13.754 | 1.00 | 24.19 | C |
| ATOM | 383 | CG2 | VAL | A | 63 | 18.620 | 26.695 | 14.692 | 1.00 | 22.51 | C |
| ATOM | 384 | N   | LEU | A | 64 | 21.007 | 23.181 | 12.756 | 1.00 | 23.15 | N |
| ATOM | 385 | CA  | LEU | A | 64 | 21.158 | 22.060 | 11.835 | 1.00 | 24.29 | C |
| ATOM | 386 | C   | LEU | A | 64 | 19.904 | 21.203 | 11.906 | 1.00 | 23.48 | C |
| ATOM | 387 | O   | LEU | A | 64 | 19.488 | 20.816 | 12.988 | 1.00 | 23.20 | O |
| ATOM | 388 | CB  | LEU | A | 64 | 22.383 | 21.235 | 12.206 | 1.00 | 24.79 | C |
| ATOM | 389 | CG  | LEU | A | 64 | 23.649 | 22.089 | 12.141 | 1.00 | 28.22 | C |
| ATOM | 390 | CD1 | LEU | A | 64 | 24.810 | 21.338 | 12.699 | 1.00 | 32.80 | C |
| ATOM | 391 | CD2 | LEU | A | 64 | 23.946 | 22.478 | 10.719 | 1.00 | 30.04 | C |
| ATOM | 392 | N   | THR | A | 65 | 19.308 | 20.910 | 10.759 | 1.00 | 22.79 | N |
| ATOM | 393 | CA  | THR | A | 65 | 18.019 | 20.218 | 10.740 | 1.00 | 23.27 | C |
| ATOM | 394 | C   | THR | A | 65 | 18.088 | 18.730 | 10.534 | 1.00 | 23.05 | C |
| ATOM | 395 | O   | THR | A | 65 | 17.102 | 18.050 | 10.765 | 1.00 | 22.85 | O |
| ATOM | 396 | CB  | THR | A | 65 | 17.150 | 20.724 | 9.571  | 1.00 | 23.53 | C |
| ATOM | 397 | OG1 | THR | A | 65 | 17.855 | 20.496 | 8.352  | 1.00 | 22.75 | O |
| ATOM | 398 | CG2 | THR | A | 65 | 16.966 | 22.226 | 9.609  | 1.00 | 24.78 | C |
| ATOM | 399 | N   | ASP | A | 66 | 19.231 | 18.227 | 10.093 | 1.00 | 23.33 | N |
| ATOM | 400 | CA  | ASP | A | 66 | 19.330 | 16.828 | 9.731  | 1.00 | 23.76 | C |
| ATOM | 401 | C   | ASP | A | 66 | 20.581 | 16.076 | 10.209 | 1.00 | 23.41 | C |
| ATOM | 402 | O   | ASP | A | 66 | 21.117 | 15.265 | 9.457  | 1.00 | 23.64 | O |
| ATOM | 403 | CB  | ASP | A | 66 | 19.245 | 16.732 | 8.199  | 1.00 | 23.97 | C |
| ATOM | 404 | CG  | ASP | A | 66 | 20.326 | 17.517 | 7.514  | 1.00 | 24.64 | C |
| ATOM | 405 | OD1 | ASP | A | 66 | 21.175 | 18.099 | 8.223  | 1.00 | 23.06 | O |
| ATOM | 406 | OD2 | ASP | A | 66 | 20.417 | 17.612 | 6.268  | 1.00 | 26.54 | O |
| ATOM | 407 | N   | THR | A | 67 | 21.050 | 16.336 | 11.428 | 1.00 | 22.72 | N |
| ATOM | 408 | CA  | THR | A | 67 | 22.235 | 15.655 | 11.912 | 1.00 | 21.85 | C |
| ATOM | 409 | C   | THR | A | 67 | 21.928 | 14.246 | 12.349 | 1.00 | 21.26 | C |
| ATOM | 410 | O   | THR | A | 67 | 22.813 | 13.429 | 12.353 | 1.00 | 20.41 | O |
| ATOM | 411 | CB  | THR | A | 67 | 22.836 | 16.345 | 13.138 | 1.00 | 21.92 | C |
| ATOM | 412 | OG1 | THR | A | 67 | 21.884 | 16.347 | 14.200 | 1.00 | 20.59 | O |
| ATOM | 413 | CG2 | THR | A | 67 | 23.161 | 17.822 | 12.873 | 1.00 | 23.29 | C |
| ATOM | 414 | N   | ASN | A | 68 | 20.684 | 13.993 | 12.752 | 1.00 | 20.82 | N |
| ATOM | 415 | CA  | ASN | A | 68 | 20.321 | 12.741 | 13.386 | 1.00 | 21.01 | C |
| ATOM | 416 | C   | ASN | A | 68 | 21.146 | 12.525 | 14.652 | 1.00 | 20.47 | C |
| ATOM | 417 | O   | ASN | A | 68 | 21.370 | 11.377 | 15.069 | 1.00 | 20.06 | O |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 418 | CB  | ASN | A | 68 | 20.516 | 11.546 | 12.444 | 1.00 | 21.63 | C |
| ATOM | 419 | CG  | ASN | A | 68 | 19.476 | 11.493 | 11.340 | 1.00 | 22.28 | C |
| ATOM | 420 | OD1 | ASN | A | 68 | 18.276 | 11.429 | 11.601 | 1.00 | 23.83 | O |
| ATOM | 421 | ND2 | ASN | A | 68 | 19.936 | 11.492 | 10.108 | 1.00 | 22.82 | N |
| ATOM | 422 | N   | LEU | A | 69 | 21.613 | 13.617 | 15.248 | 1.00 | 19.86 | N |
| ATOM | 423 | CA  | LEU | A | 69 | 22.442 | 13.533 | 16.464 | 1.00 | 19.68 | C |
| ATOM | 424 | C   | LEU | A | 69 | 21.814 | 12.707 | 17.571 | 1.00 | 19.03 | C |
| ATOM | 425 | O   | LEU | A | 69 | 22.492 | 11.878 | 18.169 | 1.00 | 18.33 | O |
| ATOM | 426 | CB  | LEU | A | 69 | 22.770 | 14.907 | 17.009 | 1.00 | 19.89 | C |
| ATOM | 427 | CG  | LEU | A | 69 | 23.654 | 14.999 | 18.239 | 1.00 | 19.87 | C |
| ATOM | 428 | CD1 | LEU | A | 69 | 24.970 | 14.289 | 18.035 | 1.00 | 20.74 | C |
| ATOM | 429 | CD2 | LEU | A | 69 | 23.911 | 16.459 | 18.577 | 1.00 | 20.41 | C |
| ATOM | 430 | N   | VAL | A | 70 | 20.538 | 12.940 | 17.860 | 1.00 | 18.84 | N |
| ATOM | 431 | CA  | VAL | A | 70 | 19.843 | 12.177 | 18.894 | 1.00 | 18.85 | C |
| ATOM | 432 | C   | VAL | A | 70 | 18.634 | 11.447 | 18.339 | 1.00 | 19.17 | C |
| ATOM | 433 | O   | VAL | A | 70 | 17.604 | 11.325 | 19.000 | 1.00 | 18.71 | O |
| ATOM | 434 | CB  | VAL | A | 70 | 19.418 | 13.038 | 20.097 | 1.00 | 18.97 | C |
| ATOM | 435 | CG1 | VAL | A | 70 | 20.645 | 13.557 | 20.812 | 1.00 | 20.41 | C |
| ATOM | 436 | CG2 | VAL | A | 70 | 18.513 | 14.185 | 19.686 | 1.00 | 18.87 | C |
| ATOM | 437 | N   | TYR | A | 71 | 18.796 | 10.916 | 17.133 | 1.00 | 20.12 | N |
| ATOM | 438 | CA  | TYR | A | 71 | 17.711 | 10.224 | 16.454 | 1.00 | 20.64 | C |
| ATOM | 439 | C   | TYR | A | 71 | 17.003 | 9.218  | 17.377 | 1.00 | 20.76 | C |
| ATOM | 440 | O   | TYR | A | 71 | 15.804 | 9.275  | 17.507 | 1.00 | 20.54 | O |
| ATOM | 441 | CB  | TYR | A | 71 | 18.186 | 9.591  | 15.136 | 1.00 | 20.75 | C |
| ATOM | 442 | CG  | TYR | A | 71 | 17.243 | 8.517  | 14.628 | 1.00 | 23.02 | C |
| ATOM | 443 | CD1 | TYR | A | 71 | 16.012 | 8.837  | 14.046 | 1.00 | 24.62 | C |
| ATOM | 444 | CD2 | TYR | A | 71 | 17.572 | 7.182  | 14.754 | 1.00 | 22.94 | C |
| ATOM | 445 | CE1 | TYR | A | 71 | 15.132 | 7.800  | 13.595 | 1.00 | 23.64 | C |
| ATOM | 446 | CE2 | TYR | A | 71 | 16.730 | 6.174  | 14.312 | 1.00 | 23.48 | C |
| ATOM | 447 | CZ  | TYR | A | 71 | 15.524 | 6.478  | 13.730 | 1.00 | 24.03 | C |
| ATOM | 448 | OH  | TYR | A | 71 | 14.697 | 5.422  | 13.349 | 1.00 | 29.55 | O |
| ATOM | 449 | N   | PRO | A | 72 | 17.728 | 8.356  | 18.068 | 1.00 | 21.35 | N |
| ATOM | 450 | CA  | PRO | A | 72 | 17.080 | 7.363  | 18.945 | 1.00 | 21.89 | C |
| ATOM | 451 | C   | PRO | A | 72 | 16.296 | 7.955  | 20.106 | 1.00 | 22.22 | C |
| ATOM | 452 | O   | PRO | A | 72 | 15.432 | 7.269  | 20.628 | 1.00 | 21.25 | O |
| ATOM | 453 | CB  | PRO | A | 72 | 18.248 | 6.538  | 19.493 | 1.00 | 21.83 | C |
| ATOM | 454 | CG  | PRO | A | 72 | 19.420 | 6.849  | 18.606 | 1.00 | 22.53 | C |
| ATOM | 455 | CD  | PRO | A | 72 | 19.192 | 8.240  | 18.080 | 1.00 | 21.81 | C |
| ATOM | 456 | N   | ALA | A | 73 | 16.568 | 9.206  | 20.484 | 1.00 | 22.77 | N |
| ATOM | 457 | CA  | ALA | A | 73 | 15.859 | 9.836  | 21.605 | 1.00 | 23.23 | C |
| ATOM | 458 | C   | ALA | A | 73 | 14.542 | 10.487 | 21.178 | 1.00 | 23.64 | C |
| ATOM | 459 | O   | ALA | A | 73 | 13.764 | 10.966 | 22.014 | 1.00 | 23.47 | O |
| ATOM | 460 | CB  | ALA | A | 73 | 16.750 | 10.860 | 22.284 | 1.00 | 22.77 | C |
| ATOM | 461 | N   | LEU | A | 74 | 14.275 | 10.507 | 19.881 | 1.00 | 24.25 | N |
| ATOM | 462 | CA  | LEU | A | 74 | 13.057 | 11.148 | 19.405 | 1.00 | 24.86 | C |
| ATOM | 463 | C   | LEU | A | 74 | 11.792 | 10.466 | 19.920 | 1.00 | 25.46 | C |
| ATOM | 464 | O   | LEU | A | 74 | 10.729 | 11.070 | 19.967 | 1.00 | 25.11 | O |
| ATOM | 465 | CB  | LEU | A | 74 | 13.055 | 11.240 | 17.881 | 1.00 | 24.77 | C |
| ATOM | 466 | CG  | LEU | A | 74 | 14.160 | 12.161 | 17.338 | 1.00 | 26.74 | C |
| ATOM | 467 | CD1 | LEU | A | 74 | 13.915 | 12.478 | 15.867 | 1.00 | 28.86 | C |
| ATOM | 468 | CD2 | LEU | A | 74 | 14.288 | 13.447 | 18.135 | 1.00 | 26.86 | C |
| ATOM | 469 | N   | LYS | A | 75 | 11.908 | 9.204  | 20.306 | 1.00 | 26.12 | N |
| ATOM | 470 | CA  | LYS | A | 75 | 10.756 | 8.460  | 20.814 | 1.00 | 26.39 | C |
| ATOM | 471 | C   | LYS | A | 75 | 10.585 | 8.687  | 22.309 | 1.00 | 26.71 | C |
| ATOM | 472 | O   | LYS | A | 75 | 9.584  | 8.284  | 22.875 | 1.00 | 26.80 | O |
| ATOM | 473 | CB  | LYS | A | 75 | 10.918 | 6.963  | 20.534 | 1.00 | 26.36 | C |
| ATOM | 474 | CG  | LYS | A | 75 | 12.141 | 6.322  | 21.185 | 1.00 | 26.49 | C |
| ATOM | 475 | CD  | LYS | A | 75 | 12.254 | 4.813  | 20.838 | 1.00 | 27.59 | C |
| ATOM | 476 | CE  | LYS | A | 75 | 13.732 | 4.367  | 20.671 | 1.00 | 27.21 | C |
| ATOM | 477 | NZ  | LYS | A | 75 | 14.475 | 4.226  | 21.912 | 1.00 | 24.71 | N |
| ATOM | 478 | N   | TRP | A | 76 | 11.561 | 9.327  | 22.950 | 1.00 | 26.64 | N |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 479 | CA  | TRP | A | 76 | 11.484 | 9.557  | 24.383 | 1.00 | 26.78 | C |
| ATOM | 480 | C   | TRP | A | 76 | 10.253 | 10.368 | 24.770 | 1.00 | 27.48 | C |
| ATOM | 481 | O   | TRP | A | 76 | 9.889  | 11.317 | 24.095 | 1.00 | 27.93 | O |
| ATOM | 482 | CB  | TRP | A | 76 | 12.717 | 10.311 | 24.888 | 1.00 | 26.57 | C |
| ATOM | 483 | CG  | TRP | A | 76 | 13.963 | 9.500  | 24.895 | 1.00 | 25.80 | C |
| ATOM | 484 | CD1 | TRP | A | 76 | 14.101 | 8.219  | 24.486 | 1.00 | 24.26 | C |
| ATOM | 485 | CD2 | TRP | A | 76 | 15.255 | 9.917  | 25.347 | 1.00 | 22.71 | C |
| ATOM | 486 | NE1 | TRP | A | 76 | 15.399 | 7.804  | 24.647 | 1.00 | 23.20 | N |
| ATOM | 487 | CE2 | TRP | A | 76 | 16.128 | 8.829  | 25.178 | 1.00 | 22.53 | C |
| ATOM | 488 | CE3 | TRP | A | 76 | 15.767 | 11.107 | 25.867 | 1.00 | 21.96 | C |
| ATOM | 489 | CZ2 | TRP | A | 76 | 17.468 | 8.890  | 25.520 | 1.00 | 22.50 | C |
| ATOM | 490 | CZ3 | TRP | A | 76 | 17.090 | 11.172 | 26.202 | 1.00 | 20.53 | C |
| ATOM | 491 | CH2 | TRP | A | 76 | 17.931 | 10.076 | 26.029 | 1.00 | 22.36 | C |
| ATOM | 492 | N   | ASP | A | 77 | 9.639  | 9.976  | 25.880 | 1.00 | 27.85 | N |
| ATOM | 493 | CA  | ASP | A | 77 | 8.532  | 10.684 | 26.484 | 1.00 | 27.74 | C |
| ATOM | 494 | C   | ASP | A | 77 | 8.560  | 10.277 | 27.957 | 1.00 | 27.45 | C |
| ATOM | 495 | O   | ASP | A | 77 | 9.373  | 9.460  | 28.336 | 1.00 | 27.22 | O |
| ATOM | 496 | CB  | ASP | A | 77 | 7.208  | 10.368 | 25.800 | 1.00 | 27.89 | C |
| ATOM | 497 | CG  | ASP | A | 77 | 6.802  | 8.913  | 25.903 | 1.00 | 29.06 | C |
| ATOM | 498 | OD1 | ASP | A | 77 | 7.354  | 8.108  | 26.708 | 1.00 | 30.51 | O |
| ATOM | 499 | OD2 | ASP | A | 77 | 5.894  | 8.489  | 25.179 | 1.00 | 31.13 | O |
| ATOM | 500 | N   | LEU | A | 78 | 7.710  | 10.847 | 28.796 | 1.00 | 27.47 | N |
| ATOM | 501 | CA  | LEU | A | 78 | 7.819  | 10.578 | 30.229 | 1.00 | 27.63 | C |
| ATOM | 502 | C   | LEU | A | 78 | 7.655  | 9.101  | 30.542 | 1.00 | 27.81 | C |
| ATOM | 503 | O   | LEU | A | 78 | 8.386  | 8.548  | 31.367 | 1.00 | 27.16 | O |
| ATOM | 504 | CB  | LEU | A | 78 | 6.818  | 11.409 | 31.011 | 1.00 | 27.59 | C |
| ATOM | 505 | CG  | LEU | A | 78 | 7.007  | 12.916 | 30.880 | 1.00 | 28.68 | C |
| ATOM | 506 | CD1 | LEU | A | 78 | 5.906  | 13.677 | 31.612 | 1.00 | 28.95 | C |
| ATOM | 507 | CD2 | LEU | A | 78 | 8.369  | 13.328 | 31.412 | 1.00 | 29.32 | C |
| ATOM | 508 | N   | GLU | A | 79 | 6.721  | 8.450  | 29.860 | 1.00 | 28.17 | N |
| ATOM | 509 | CA  | GLU | A | 79 | 6.480  | 7.035  | 30.102 | 1.00 | 28.56 | C |
| ATOM | 510 | C   | GLU | A | 79 | 7.715  | 6.185  | 29.781 | 1.00 | 28.22 | C |
| ATOM | 511 | O   | GLU | A | 79 | 8.167  | 5.388  | 30.600 | 1.00 | 27.73 | O |
| ATOM | 512 | CB  | GLU | A | 79 | 5.267  | 6.540  | 29.298 | 1.00 | 28.87 | C |
| ATOM | 513 | CG  | GLU | A | 79 | 5.051  | 5.049  | 29.467 | 1.00 | 31.45 | C |
| ATOM | 514 | CD  | GLU | A | 79 | 3.849  | 4.516  | 28.716 | 1.00 | 34.79 | C |
| ATOM | 515 | OE1 | GLU | A | 79 | 3.422  | 5.129  | 27.709 | 1.00 | 35.78 | O |
| ATOM | 516 | OE2 | GLU | A | 79 | 3.343  | 3.457  | 29.144 | 1.00 | 37.92 | O |
| ATOM | 517 | N   | TYR | A | 80 | 8.260  | 6.346  | 28.582 | 1.00 | 28.27 | N |
| ATOM | 518 | CA  | TYR | A | 80 | 9.452  | 5.597  | 28.200 | 1.00 | 28.00 | C |
| ATOM | 519 | C   | TYR | A | 80 | 10.628 | 5.873  | 29.142 | 1.00 | 27.64 | C |
| ATOM | 520 | O   | TYR | A | 80 | 11.330 | 4.958  | 29.563 | 1.00 | 27.16 | O |
| ATOM | 521 | CB  | TYR | A | 80 | 9.838  | 5.964  | 26.787 | 1.00 | 28.13 | C |
| ATOM | 522 | CG  | TYR | A | 80 | 11.054 | 5.250  | 26.246 | 1.00 | 27.95 | C |
| ATOM | 523 | CD1 | TYR | A | 80 | 10.952 | 3.991  | 25.644 | 1.00 | 27.39 | C |
| ATOM | 524 | CD2 | TYR | A | 80 | 12.300 | 5.846  | 26.306 | 1.00 | 25.55 | C |
| ATOM | 525 | CE1 | TYR | A | 80 | 12.089 | 3.352  | 25.128 | 1.00 | 26.82 | C |
| ATOM | 526 | CE2 | TYR | A | 80 | 13.417 | 5.224  | 25.808 | 1.00 | 25.50 | C |
| ATOM | 527 | CZ  | TYR | A | 80 | 13.320 | 3.992  | 25.213 | 1.00 | 25.64 | C |
| ATOM | 528 | OH  | TYR | A | 80 | 14.467 | 3.426  | 24.703 | 1.00 | 23.50 | O |
| ATOM | 529 | N   | LEU | A | 81 | 10.839 | 7.135  | 29.482 | 1.00 | 27.51 | N |
| ATOM | 530 | CA  | LEU | A | 81 | 11.952 | 7.477  | 30.371 | 1.00 | 27.75 | C |
| ATOM | 531 | C   | LEU | A | 81 | 11.741 | 6.943  | 31.801 | 1.00 | 27.76 | C |
| ATOM | 532 | O   | LEU | A | 81 | 12.682 | 6.459  | 32.437 | 1.00 | 27.35 | O |
| ATOM | 533 | CB  | LEU | A | 81 | 12.194 | 8.990  | 30.399 | 1.00 | 27.35 | C |
| ATOM | 534 | CG  | LEU | A | 81 | 12.659 | 9.656  | 29.096 | 1.00 | 28.06 | C |
| ATOM | 535 | CD1 | LEU | A | 81 | 12.664 | 11.170 | 29.269 | 1.00 | 28.55 | C |
| ATOM | 536 | CD2 | LEU | A | 81 | 14.036 | 9.192  | 28.655 | 1.00 | 27.65 | C |
| ATOM | 537 | N   | GLN | A | 82 | 10.521 | 7.049  | 32.313 | 1.00 | 28.10 | N |
| ATOM | 538 | CA  | GLN | A | 82 | 10.234 | 6.557  | 33.656 | 1.00 | 28.61 | C |
| ATOM | 539 | C   | GLN | A | 82 | 10.525 | 5.066  | 33.689 | 1.00 | 28.32 | C |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 540 | O   | GLN | A | 82 | 11.070 | 4.550  | 34.643 | 1.00 | 28.25 | O |
| ATOM | 541 | CB  | GLN | A | 82 | 8.774  | 6.805  | 34.032 | 1.00 | 29.04 | C |
| ATOM | 542 | CG  | GLN | A | 82 | 8.325  | 6.063  | 35.293 | 1.00 | 30.18 | C |
| ATOM | 543 | CD  | GLN | A | 82 | 7.184  | 6.754  | 36.042 | 1.00 | 32.25 | C |
| ATOM | 544 | OE1 | GLN | A | 82 | 6.642  | 7.758  | 35.594 | 1.00 | 34.51 | O |
| ATOM | 545 | NE2 | GLN | A | 82 | 6.822  | 6.204  | 37.189 | 1.00 | 36.79 | N |
| ATOM | 546 | N   | GLU | A | 83 | 10.193 | 4.397  | 32.601 | 1.00 | 28.58 | N |
| ATOM | 547 | CA  | GLU | A | 83 | 10.349 | 2.950  | 32.492 | 1.00 | 28.70 | C |
| ATOM | 548 | C   | GLU | A | 83 | 11.801 | 2.515  | 32.314 | 1.00 | 28.14 | C |
| ATOM | 549 | O   | GLU | A | 83 | 12.166 | 1.424  | 32.713 | 1.00 | 27.54 | O |
| ATOM | 550 | CB  | GLU | A | 83 | 9.506  | 2.438  | 31.319 | 1.00 | 28.53 | C |
| ATOM | 551 | CG  | GLU | A | 83 | 9.562  | 0.937  | 31.101 | 1.00 | 30.76 | C |
| ATOM | 552 | CD  | GLU | A | 83 | 8.985  | 0.150  | 32.265 | 1.00 | 33.31 | C |
| ATOM | 553 | OE1 | GLU | A | 83 | 8.172  | 0.713  | 33.030 | 1.00 | 35.22 | O |
| ATOM | 554 | OE2 | GLU | A | 83 | 9.352  | -1.033 | 32.428 | 1.00 | 35.98 | O |
| ATOM | 555 | N   | ASN | A | 84 | 12.644 | 3.374  | 31.753 | 1.00 | 27.44 | N |
| ATOM | 556 | CA  | ASN | A | 84 | 13.985 | 2.938  | 31.400 | 1.00 | 27.09 | C |
| ATOM | 557 | C   | ASN | A | 84 | 15.168 | 3.729  | 31.913 | 1.00 | 27.31 | C |
| ATOM | 558 | O   | ASN | A | 84 | 16.291 | 3.276  | 31.759 | 1.00 | 27.17 | O |
| ATOM | 559 | CB  | ASN | A | 84 | 14.099 | 2.917  | 29.879 | 1.00 | 27.17 | C |
| ATOM | 560 | CG  | ASN | A | 84 | 13.226 | 1.890  | 29.254 | 1.00 | 26.24 | C |
| ATOM | 561 | OD1 | ASN | A | 84 | 13.361 | 0.696  | 29.532 | 1.00 | 27.49 | O |
| ATOM | 562 | ND2 | ASN | A | 84 | 12.312 | 2.333  | 28.413 | 1.00 | 23.37 | N |
| ATOM | 563 | N   | ILE | A | 85 | 14.952 | 4.893  | 32.511 | 1.00 | 27.52 | N |
| ATOM | 564 | CA  | ILE | A | 85 | 16.088 | 5.734  | 32.861 | 1.00 | 28.25 | C |
| ATOM | 565 | C   | ILE | A | 85 | 16.788 | 5.390  | 34.185 | 1.00 | 28.03 | C |
| ATOM | 566 | O   | ILE | A | 85 | 17.700 | 6.094  | 34.610 | 1.00 | 28.40 | O |
| ATOM | 567 | CB  | ILE | A | 85 | 15.684 | 7.221  | 32.801 | 1.00 | 28.23 | C |
| ATOM | 568 | CG1 | ILE | A | 85 | 16.872 | 8.069  | 32.342 | 1.00 | 29.61 | C |
| ATOM | 569 | CG2 | ILE | A | 85 | 15.143 | 7.694  | 34.139 | 1.00 | 29.11 | C |
| ATOM | 570 | CD1 | ILE | A | 85 | 16.520 | 9.535  | 31.996 | 1.00 | 28.97 | C |
| ATOM | 571 | N   | GLY | A | 86 | 16.368 | 4.317  | 34.833 | 1.00 | 28.14 | N |
| ATOM | 572 | CA  | GLY | A | 86 | 17.014 | 3.874  | 36.061 | 1.00 | 28.15 | C |
| ATOM | 573 | C   | GLY | A | 86 | 16.478 | 4.504  | 37.335 | 1.00 | 28.11 | C |
| ATOM | 574 | O   | GLY | A | 86 | 15.494 | 5.251  | 37.308 | 1.00 | 27.93 | O |
| ATOM | 575 | N   | ASN | A | 87 | 17.162 | 4.220  | 38.444 | 1.00 | 27.96 | N |
| ATOM | 576 | CA  | ASN | A | 87 | 16.754 | 4.672  | 39.767 | 1.00 | 27.88 | C |
| ATOM | 577 | C   | ASN | A | 87 | 17.736 | 5.677  | 40.373 | 1.00 | 27.82 | C |
| ATOM | 578 | O   | ASN | A | 87 | 17.751 | 5.886  | 41.585 | 1.00 | 27.63 | O |
| ATOM | 579 | CB  | ASN | A | 87 | 16.571 | 3.447  | 40.713 | 1.00 | 27.89 | C |
| ATOM | 580 | N   | GLY | A | 88 | 18.559 | 6.301  | 39.538 | 1.00 | 28.21 | N |
| ATOM | 581 | CA  | GLY | A | 88 | 19.478 | 7.336  | 40.006 | 1.00 | 28.18 | C |
| ATOM | 582 | C   | GLY | A | 88 | 18.706 | 8.584  | 40.396 | 1.00 | 28.19 | C |
| ATOM | 583 | O   | GLY | A | 88 | 17.520 | 8.676  | 40.097 | 1.00 | 28.62 | O |
| ATOM | 584 | N   | ASP | A | 89 | 19.357 | 9.530  | 41.068 | 1.00 | 27.99 | N |
| ATOM | 585 | CA  | ASP | A | 89 | 18.707 | 10.781 | 41.468 | 1.00 | 28.09 | C |
| ATOM | 586 | C   | ASP | A | 89 | 18.655 | 11.806 | 40.335 | 1.00 | 28.00 | C |
| ATOM | 587 | O   | ASP | A | 89 | 19.557 | 11.866 | 39.507 | 1.00 | 28.07 | O |
| ATOM | 588 | CB  | ASP | A | 89 | 19.467 | 11.433 | 42.613 | 1.00 | 28.24 | C |
| ATOM | 589 | CG  | ASP | A | 89 | 19.249 | 10.747 | 43.935 | 1.00 | 28.53 | C |
| ATOM | 590 | OD1 | ASP | A | 89 | 18.398 | 9.843  | 44.024 | 1.00 | 30.26 | O |
| ATOM | 591 | OD2 | ASP | A | 89 | 19.884 | 11.070 | 44.955 | 1.00 | 29.31 | O |
| ATOM | 592 | N   | PHE | A | 90 | 17.620 | 12.637 | 40.330 | 1.00 | 27.56 | N |
| ATOM | 593 | CA  | PHE | A | 90 | 17.510 | 13.687 | 39.332 | 1.00 | 27.37 | C |
| ATOM | 594 | C   | PHE | A | 90 | 17.291 | 15.037 | 39.993 | 1.00 | 27.78 | C |
| ATOM | 595 | O   | PHE | A | 90 | 16.453 | 15.171 | 40.884 | 1.00 | 27.69 | O |
| ATOM | 596 | CB  | PHE | A | 90 | 16.378 | 13.388 | 38.351 | 1.00 | 27.05 | C |
| ATOM | 597 | CG  | PHE | A | 90 | 16.678 | 12.262 | 37.408 | 1.00 | 25.85 | C |
| ATOM | 598 | CD1 | PHE | A | 90 | 16.525 | 10.943 | 37.806 | 1.00 | 25.70 | C |
| ATOM | 599 | CD2 | PHE | A | 90 | 17.119 | 12.521 | 36.121 | 1.00 | 26.20 | C |
| ATOM | 600 | CE1 | PHE | A | 90 | 16.797 | 9.908  | 36.943 | 1.00 | 24.06 | C |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 601 | CE2 | PHE | A | 90 | 17.395 | 11.489 | 35.248 | 1.00 | 25.49 | C |
| ATOM | 602 | CZ  | PHE | A | 90 | 17.235 | 10.176 | 35.666 | 1.00 | 25.33 | C |
| ATOM | 603 | N   | SER | A | 91 | 18.062 | 16.033 | 39.560 | 1.00 | 27.85 | N |
| ATOM | 604 | CA  | SER | A | 91 | 17.902 | 17.384 | 40.075 | 1.00 | 28.17 | C |
| ATOM | 605 | C   | SER | A | 91 | 16.695 | 18.023 | 39.419 | 1.00 | 28.48 | C |
| ATOM | 606 | O   | SER | A | 91 | 16.589 | 18.085 | 38.192 | 1.00 | 28.35 | O |
| ATOM | 607 | CB  | SER | A | 91 | 19.149 | 18.236 | 39.838 | 1.00 | 27.86 | C |
| ATOM | 608 | OG  | SER | A | 91 | 20.260 | 17.652 | 40.485 | 1.00 | 27.15 | O |
| ATOM | 609 | N   | VAL | A | 92 | 15.784 | 18.482 | 40.261 | 1.00 | 29.05 | N |
| ATOM | 610 | CA  | VAL | A | 92 | 14.585 | 19.141 | 39.812 | 1.00 | 29.67 | C |
| ATOM | 611 | C   | VAL | A | 92 | 14.437 | 20.465 | 40.529 | 1.00 | 30.31 | C |
| ATOM | 612 | O   | VAL | A | 92 | 14.442 | 20.537 | 41.763 | 1.00 | 30.37 | O |
| ATOM | 613 | CB  | VAL | A | 92 | 13.352 | 18.313 | 40.106 | 1.00 | 29.81 | C |
| ATOM | 614 | CG1 | VAL | A | 92 | 12.106 | 19.026 | 39.582 | 1.00 | 29.93 | C |
| ATOM | 615 | CG2 | VAL | A | 92 | 13.490 | 16.930 | 39.507 | 1.00 | 29.60 | C |
| ATOM | 616 | N   | TYR | A | 93 | 14.329 | 21.516 | 39.732 | 1.00 | 31.00 | N |
| ATOM | 617 | CA  | TYR | A | 93 | 14.135 | 22.845 | 40.241 | 1.00 | 31.29 | C |
| ATOM | 618 | C   | TYR | A | 93 | 12.662 | 23.113 | 40.298 | 1.00 | 31.54 | C |
| ATOM | 619 | O   | TYR | A | 93 | 11.892 | 22.701 | 39.423 | 1.00 | 31.35 | O |
| ATOM | 620 | CB  | TYR | A | 93 | 14.829 | 23.853 | 39.345 | 1.00 | 31.87 | C |
| ATOM | 621 | CG  | TYR | A | 93 | 16.310 | 23.711 | 39.436 | 1.00 | 33.05 | C |
| ATOM | 622 | CD1 | TYR | A | 93 | 17.012 | 24.283 | 40.482 | 1.00 | 34.67 | C |
| ATOM | 623 | CD2 | TYR | A | 93 | 16.998 | 22.954 | 38.525 | 1.00 | 34.24 | C |
| ATOM | 624 | CE1 | TYR | A | 93 | 18.357 | 24.125 | 40.593 | 1.00 | 35.09 | C |
| ATOM | 625 | CE2 | TYR | A | 93 | 18.338 | 22.789 | 38.634 | 1.00 | 36.36 | C |
| ATOM | 626 | CZ  | TYR | A | 93 | 19.011 | 23.379 | 39.670 | 1.00 | 36.33 | C |
| ATOM | 627 | OH  | TYR | A | 93 | 20.357 | 23.204 | 39.772 | 1.00 | 40.81 | O |
| ATOM | 628 | N   | SER | A | 94 | 12.286 | 23.813 | 41.351 | 1.00 | 32.03 | N |
| ATOM | 629 | CA  | SER | A | 94 | 10.919 | 24.182 | 41.599 | 1.00 | 32.31 | C |
| ATOM | 630 | C   | SER | A | 94 | 10.884 | 25.692 | 41.704 | 1.00 | 32.42 | C |
| ATOM | 631 | O   | SER | A | 94 | 11.743 | 26.286 | 42.350 | 1.00 | 32.48 | O |
| ATOM | 632 | CB  | SER | A | 94 | 10.464 | 23.566 | 42.914 | 1.00 | 32.38 | C |
| ATOM | 633 | OG  | SER | A | 94 | 9.062  | 23.691 | 43.052 | 1.00 | 33.53 | O |
| ATOM | 634 | N   | ALA | A | 95 | 9.902  | 26.314 | 41.070 | 1.00 | 32.58 | N |
| ATOM | 635 | CA  | ALA | A | 95 | 9.766  | 27.757 | 41.135 | 1.00 | 32.90 | C |
| ATOM | 636 | C   | ALA | A | 95 | 8.312  | 28.172 | 41.076 | 1.00 | 33.48 | C |
| ATOM | 637 | O   | ALA | A | 95 | 7.446  | 27.429 | 40.620 | 1.00 | 33.62 | O |
| ATOM | 638 | CB  | ALA | A | 95 | 10.528 | 28.413 | 39.996 | 1.00 | 32.80 | C |
| ATOM | 639 | N   | SER | A | 96 | 8.053  | 29.382 | 41.539 | 1.00 | 34.08 | N |
| ATOM | 640 | CA  | SER | A | 96 | 6.721  | 29.932 | 41.482 | 1.00 | 34.75 | C |
| ATOM | 641 | C   | SER | A | 96 | 6.616  | 30.974 | 40.382 | 1.00 | 34.55 | C |
| ATOM | 642 | O   | SER | A | 96 | 5.603  | 31.659 | 40.275 | 1.00 | 35.29 | O |
| ATOM | 643 | CB  | SER | A | 96 | 6.363  | 30.592 | 42.801 | 1.00 | 35.05 | C |
| ATOM | 644 | OG  | SER | A | 96 | 5.165  | 31.311 | 42.627 | 1.00 | 36.18 | O |
| ATOM | 645 | N   | THR | A | 97 | 7.673  | 31.107 | 39.593 | 1.00 | 33.88 | N |
| ATOM | 646 | CA  | THR | A | 97 | 7.716  | 32.046 | 38.477 | 1.00 | 33.41 | C |
| ATOM | 647 | C   | THR | A | 97 | 8.084  | 31.238 | 37.265 | 1.00 | 32.32 | C |
| ATOM | 648 | O   | THR | A | 97 | 8.590  | 30.143 | 37.411 | 1.00 | 32.10 | O |
| ATOM | 649 | CB  | THR | A | 97 | 8.797  | 33.144 | 38.695 | 1.00 | 33.64 | C |
| ATOM | 650 | OG1 | THR | A | 97 | 9.067  | 33.810 | 37.460 | 1.00 | 33.76 | O |
| ATOM | 651 | CG2 | THR | A | 97 | 10.190 | 32.559 | 39.058 | 1.00 | 34.25 | C |
| ATOM | 652 | N   | HIS | A | 98 | 7.840  | 31.762 | 36.073 | 1.00 | 31.47 | N |
| ATOM | 653 | CA  | HIS | A | 98 | 8.278  | 31.071 | 34.863 | 1.00 | 30.97 | C |
| ATOM | 654 | C   | HIS | A | 98 | 9.804  | 31.134 | 34.707 | 1.00 | 30.53 | C |
| ATOM | 655 | O   | HIS | A | 98 | 10.378 | 30.379 | 33.940 | 1.00 | 29.14 | O |
| ATOM | 656 | CB  | HIS | A | 98 | 7.613  | 31.666 | 33.621 | 1.00 | 31.14 | C |
| ATOM | 657 | CG  | HIS | A | 98 | 7.878  | 33.125 | 33.415 | 1.00 | 30.86 | C |
| ATOM | 658 | ND1 | HIS | A | 98 | 7.121  | 34.112 | 34.011 | 1.00 | 31.51 | N |
| ATOM | 659 | CD2 | HIS | A | 98 | 8.795  | 33.767 | 32.651 | 1.00 | 31.48 | C |
| ATOM | 660 | CE1 | HIS | A | 98 | 7.566  | 35.298 | 33.634 | 1.00 | 31.14 | C |
| ATOM | 661 | NE2 | HIS | A | 98 | 8.581  | 35.118 | 32.805 | 1.00 | 30.50 | N |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 662 | N   | LYS | A | 99  | 10.459 | 32.025 | 35.449 | 1.00 | 30.36 | N |
| ATOM | 663 | CA  | LYS | A | 99  | 11.895 | 32.198 | 35.298 | 1.00 | 31.07 | C |
| ATOM | 664 | C   | LYS | A | 99  | 12.761 | 31.288 | 36.166 | 1.00 | 31.00 | C |
| ATOM | 665 | O   | LYS | A | 99  | 12.693 | 31.337 | 37.396 | 1.00 | 31.91 | O |
| ATOM | 666 | CB  | LYS | A | 99  | 12.265 | 33.643 | 35.544 | 1.00 | 31.15 | C |
| ATOM | 667 | CG  | LYS | A | 99  | 11.887 | 34.551 | 34.391 | 1.00 | 33.39 | C |
| ATOM | 668 | CD  | LYS | A | 99  | 12.486 | 35.945 | 34.556 | 1.00 | 36.16 | C |
| ATOM | 669 | CE  | LYS | A | 99  | 11.763 | 36.771 | 35.607 | 1.00 | 37.52 | C |
| ATOM | 670 | NZ  | LYS | A | 99  | 10.620 | 37.507 | 35.006 | 1.00 | 38.84 | N |
| ATOM | 671 | N   | PHE | A | 100 | 13.572 | 30.453 | 35.518 | 1.00 | 30.20 | N |
| ATOM | 672 | CA  | PHE | A | 100 | 14.517 | 29.606 | 36.232 | 1.00 | 30.03 | C |
| ATOM | 673 | C   | PHE | A | 100 | 15.952 | 30.123 | 36.138 | 1.00 | 29.72 | C |
| ATOM | 674 | O   | PHE | A | 100 | 16.826 | 29.544 | 35.481 | 1.00 | 29.39 | O |
| ATOM | 675 | CB  | PHE | A | 100 | 14.441 | 28.168 | 35.744 | 1.00 | 29.93 | C |
| ATOM | 676 | CG  | PHE | A | 100 | 13.223 | 27.452 | 36.206 | 1.00 | 29.72 | C |
| ATOM | 677 | CD1 | PHE | A | 100 | 12.014 | 27.637 | 35.566 | 1.00 | 28.98 | C |
| ATOM | 678 | CD2 | PHE | A | 100 | 13.283 | 26.596 | 37.289 | 1.00 | 30.77 | C |
| ATOM | 679 | CE1 | PHE | A | 100 | 10.896 | 26.969 | 35.983 | 1.00 | 30.22 | C |
| ATOM | 680 | CE2 | PHE | A | 100 | 12.158 | 25.919 | 37.719 | 1.00 | 30.51 | C |
| ATOM | 681 | CZ  | PHE | A | 100 | 10.967 | 26.105 | 37.069 | 1.00 | 30.63 | C |
| ATOM | 682 | N   | LEU | A | 101 | 16.178 | 31.235 | 36.809 | 1.00 | 29.87 | N |
| ATOM | 683 | CA  | LEU | A | 101 | 17.495 | 31.812 | 36.919 | 1.00 | 29.57 | C |
| ATOM | 684 | C   | LEU | A | 101 | 18.451 | 30.814 | 37.555 | 1.00 | 29.61 | C |
| ATOM | 685 | O   | LEU | A | 101 | 18.249 | 30.380 | 38.679 | 1.00 | 28.35 | O |
| ATOM | 686 | CB  | LEU | A | 101 | 17.412 | 33.057 | 37.787 | 1.00 | 29.68 | C |
| ATOM | 687 | CG  | LEU | A | 101 | 18.707 | 33.845 | 37.954 | 1.00 | 29.68 | C |
| ATOM | 688 | CD1 | LEU | A | 101 | 19.184 | 34.337 | 36.620 | 1.00 | 28.70 | C |
| ATOM | 689 | CD2 | LEU | A | 101 | 18.474 | 35.014 | 38.909 | 1.00 | 31.41 | C |
| ATOM | 690 | N   | TYR | A | 102 | 19.490 | 30.440 | 36.816 | 1.00 | 30.36 | N |
| ATOM | 691 | CA  | TYR | A | 102 | 20.516 | 29.535 | 37.338 | 1.00 | 30.64 | C |
| ATOM | 692 | C   | TYR | A | 102 | 21.332 | 30.228 | 38.440 | 1.00 | 30.93 | C |
| ATOM | 693 | O   | TYR | A | 102 | 21.623 | 31.425 | 38.339 | 1.00 | 30.67 | O |
| ATOM | 694 | CB  | TYR | A | 102 | 21.480 | 29.101 | 36.224 | 1.00 | 30.45 | C |
| ATOM | 695 | CG  | TYR | A | 102 | 22.609 | 28.271 | 36.774 | 1.00 | 31.25 | C |
| ATOM | 696 | CD1 | TYR | A | 102 | 22.430 | 26.916 | 37.062 | 1.00 | 31.33 | C |
| ATOM | 697 | CD2 | TYR | A | 102 | 23.842 | 28.844 | 37.054 | 1.00 | 31.29 | C |
| ATOM | 698 | CE1 | TYR | A | 102 | 23.456 | 26.163 | 37.612 | 1.00 | 32.81 | C |
| ATOM | 699 | CE2 | TYR | A | 102 | 24.869 | 28.098 | 37.601 | 1.00 | 32.24 | C |
| ATOM | 700 | CZ  | TYR | A | 102 | 24.676 | 26.764 | 37.876 | 1.00 | 34.18 | C |
| ATOM | 701 | OH  | TYR | A | 102 | 25.720 | 26.030 | 38.418 | 1.00 | 39.06 | O |
| ATOM | 702 | N   | TYR | A | 103 | 21.684 | 29.478 | 39.488 | 1.00 | 31.28 | N |
| ATOM | 703 | CA  | TYR | A | 103 | 22.569 | 29.983 | 40.539 | 1.00 | 31.56 | C |
| ATOM | 704 | C   | TYR | A | 103 | 23.524 | 28.911 | 41.058 | 1.00 | 31.11 | C |
| ATOM | 705 | O   | TYR | A | 103 | 23.190 | 27.732 | 41.165 | 1.00 | 30.75 | O |
| ATOM | 706 | CB  | TYR | A | 103 | 21.796 | 30.599 | 41.706 | 1.00 | 31.98 | C |
| ATOM | 707 | CG  | TYR | A | 103 | 20.846 | 29.663 | 42.385 | 1.00 | 33.92 | C |
| ATOM | 708 | CD1 | TYR | A | 103 | 19.577 | 29.445 | 41.868 | 1.00 | 36.08 | C |
| ATOM | 709 | CD2 | TYR | A | 103 | 21.203 | 29.010 | 43.553 | 1.00 | 36.91 | C |
| ATOM | 710 | CE1 | TYR | A | 103 | 18.696 | 28.587 | 42.483 | 1.00 | 37.42 | C |
| ATOM | 711 | CE2 | TYR | A | 103 | 20.325 | 28.153 | 44.189 | 1.00 | 37.63 | C |
| ATOM | 712 | CZ  | TYR | A | 103 | 19.070 | 27.947 | 43.647 | 1.00 | 38.74 | C |
| ATOM | 713 | OH  | TYR | A | 103 | 18.183 | 27.099 | 44.264 | 1.00 | 40.90 | O |
| ATOM | 714 | N   | ASP | A | 104 | 24.725 | 29.345 | 41.391 | 1.00 | 30.34 | N |
| ATOM | 715 | CA  | ASP | A | 104 | 25.752 | 28.444 | 41.873 | 1.00 | 30.04 | C |
| ATOM | 716 | C   | ASP | A | 104 | 25.735 | 28.408 | 43.394 | 1.00 | 29.73 | C |
| ATOM | 717 | O   | ASP | A | 104 | 26.079 | 29.388 | 44.062 | 1.00 | 28.53 | O |
| ATOM | 718 | CB  | ASP | A | 104 | 27.089 | 28.931 | 41.350 | 1.00 | 30.07 | C |
| ATOM | 719 | CG  | ASP | A | 104 | 28.233 | 28.037 | 41.731 | 1.00 | 30.02 | C |
| ATOM | 720 | OD1 | ASP | A | 104 | 28.069 | 27.137 | 42.605 | 1.00 | 28.92 | O |
| ATOM | 721 | OD2 | ASP | A | 104 | 29.339 | 28.183 | 41.168 | 1.00 | 29.24 | O |
| ATOM | 722 | N   | GLU | A | 105 | 25.327 | 27.263 | 43.931 | 1.00 | 29.74 | N |



|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 723 | CA  | GLU | A | 105 | 25.169 | 27.095 | 45.371 | 1.00 | 29.91 | C |
| ATOM | 724 | C   | GLU | A | 105 | 26.461 | 27.343 | 46.155 | 1.00 | 29.29 | C |
| ATOM | 725 | O   | GLU | A | 105 | 26.412 | 27.872 | 47.263 | 1.00 | 28.37 | O |
| ATOM | 726 | CB  | GLU | A | 105 | 24.601 | 25.699 | 45.672 | 1.00 | 30.40 | C |
| ATOM | 727 | CG  | GLU | A | 105 | 23.097 | 25.621 | 45.410 | 1.00 | 32.58 | C |
| ATOM | 728 | CD  | GLU | A | 105 | 22.546 | 24.210 | 45.287 | 1.00 | 34.72 | C |
| ATOM | 729 | OE1 | GLU | A | 105 | 22.945 | 23.320 | 46.072 | 1.00 | 35.38 | O |
| ATOM | 730 | OE2 | GLU | A | 105 | 21.683 | 24.001 | 44.402 | 1.00 | 35.93 | O |
| ATOM | 731 | N   | LYS | A | 106 | 27.607 | 27.000 | 45.565 | 1.00 | 29.02 | N |
| ATOM | 732 | CA  | LYS | A | 106 | 28.897 | 27.156 | 46.243 | 1.00 | 29.26 | C |
| ATOM | 733 | C   | LYS | A | 106 | 29.245 | 28.608 | 46.493 | 1.00 | 29.31 | C |
| ATOM | 734 | O   | LYS | A | 106 | 30.051 | 28.903 | 47.363 | 1.00 | 28.83 | O |
| ATOM | 735 | CB  | LYS | A | 106 | 30.036 | 26.530 | 45.433 | 1.00 | 29.60 | C |
| ATOM | 736 | CG  | LYS | A | 106 | 29.864 | 25.036 | 45.094 | 1.00 | 30.18 | C |
| ATOM | 737 | N   | LYS | A | 107 | 28.646 | 29.516 | 45.724 | 1.00 | 29.27 | N |
| ATOM | 738 | CA  | LYS | A | 107 | 28.925 | 30.933 | 45.876 | 1.00 | 29.61 | C |
| ATOM | 739 | C   | LYS | A | 107 | 27.933 | 31.605 | 46.820 | 1.00 | 30.29 | C |
| ATOM | 740 | O   | LYS | A | 107 | 28.062 | 32.785 | 47.100 | 1.00 | 30.16 | O |
| ATOM | 741 | CB  | LYS | A | 107 | 28.924 | 31.636 | 44.504 | 1.00 | 29.35 | C |
| ATOM | 742 | CG  | LYS | A | 107 | 30.222 | 31.411 | 43.697 | 1.00 | 28.97 | C |
| ATOM | 743 | CD  | LYS | A | 107 | 30.142 | 31.864 | 42.230 | 1.00 | 26.18 | C |
| ATOM | 744 | CE  | LYS | A | 107 | 31.459 | 31.534 | 41.498 | 1.00 | 26.51 | C |
| ATOM | 745 | NZ  | LYS | A | 107 | 31.578 | 32.052 | 40.083 | 1.00 | 24.21 | N |
| ATOM | 746 | N   | MET | A | 108 | 26.950 | 30.869 | 47.320 | 1.00 | 31.39 | N |
| ATOM | 747 | CA  | MET | A | 108 | 25.939 | 31.482 | 48.186 | 1.00 | 32.74 | C |
| ATOM | 748 | C   | MET | A | 108 | 26.468 | 32.050 | 49.514 | 1.00 | 33.50 | C |
| ATOM | 749 | O   | MET | A | 108 | 25.987 | 33.082 | 49.988 | 1.00 | 33.27 | O |
| ATOM | 750 | CB  | MET | A | 108 | 24.787 | 30.509 | 48.417 | 1.00 | 33.11 | C |
| ATOM | 751 | CG  | MET | A | 108 | 23.976 | 30.300 | 47.127 | 1.00 | 34.43 | C |
| ATOM | 752 | SD  | MET | A | 108 | 22.458 | 29.330 | 47.263 | 1.00 | 37.47 | S |
| ATOM | 753 | CE  | MET | A | 108 | 21.487 | 30.326 | 48.417 | 1.00 | 37.24 | C |
| ATOM | 754 | N   | ALA | A | 109 | 27.484 | 31.427 | 50.090 | 1.00 | 34.73 | N |
| ATOM | 755 | CA  | ALA | A | 109 | 28.039 | 31.922 | 51.359 | 1.00 | 36.13 | C |
| ATOM | 756 | C   | ALA | A | 109 | 28.555 | 33.361 | 51.266 | 1.00 | 37.12 | C |
| ATOM | 757 | O   | ALA | A | 109 | 28.455 | 34.127 | 52.213 | 1.00 | 37.35 | O |
| ATOM | 758 | CB  | ALA | A | 109 | 29.147 | 30.991 | 51.860 | 1.00 | 35.96 | C |
| ATOM | 759 | N   | ASN | A | 110 | 29.076 | 33.745 | 50.112 | 1.00 | 38.70 | N |
| ATOM | 760 | CA  | ASN | A | 110 | 29.631 | 35.090 | 49.949 | 1.00 | 39.61 | C |
| ATOM | 761 | C   | ASN | A | 110 | 28.605 | 36.188 | 49.621 | 1.00 | 39.61 | C |
| ATOM | 762 | O   | ASN | A | 110 | 28.950 | 37.359 | 49.500 | 1.00 | 39.50 | O |
| ATOM | 763 | CB  | ASN | A | 110 | 30.730 | 35.036 | 48.888 | 1.00 | 39.94 | C |
| ATOM | 764 | CG  | ASN | A | 110 | 31.916 | 34.186 | 49.329 | 1.00 | 41.54 | C |
| ATOM | 765 | OD1 | ASN | A | 110 | 32.341 | 34.223 | 50.503 | 1.00 | 41.36 | O |
| ATOM | 766 | ND2 | ASN | A | 110 | 32.451 | 33.406 | 48.399 | 1.00 | 43.06 | N |
| ATOM | 767 | N   | PHE | A | 111 | 27.349 | 35.802 | 49.465 | 1.00 | 40.12 | N |
| ATOM | 768 | CA  | PHE | A | 111 | 26.278 | 36.753 | 49.208 | 1.00 | 40.43 | C |
| ATOM | 769 | C   | PHE | A | 111 | 25.064 | 36.292 | 50.016 | 1.00 | 41.38 | C |
| ATOM | 770 | O   | PHE | A | 111 | 24.068 | 35.811 | 49.471 | 1.00 | 40.89 | O |
| ATOM | 771 | CB  | PHE | A | 111 | 25.954 | 36.839 | 47.710 | 1.00 | 40.30 | C |
| ATOM | 772 | CG  | PHE | A | 111 | 26.973 | 37.597 | 46.910 | 1.00 | 38.60 | C |
| ATOM | 773 | CD1 | PHE | A | 111 | 28.199 | 37.033 | 46.618 | 1.00 | 37.50 | C |
| ATOM | 774 | CD2 | PHE | A | 111 | 26.705 | 38.867 | 46.445 | 1.00 | 38.02 | C |
| ATOM | 775 | CE1 | PHE | A | 111 | 29.140 | 37.725 | 45.890 | 1.00 | 36.74 | C |
| ATOM | 776 | CE2 | PHE | A | 111 | 27.649 | 39.560 | 45.705 | 1.00 | 36.60 | C |
| ATOM | 777 | CZ  | PHE | A | 111 | 28.863 | 38.986 | 45.433 | 1.00 | 35.45 | C |
| ATOM | 778 | N   | GLN | A | 112 | 25.175 | 36.457 | 51.329 | 1.00 | 42.72 | N |
| ATOM | 779 | CA  | GLN | A | 112 | 24.154 | 36.022 | 52.276 | 1.00 | 43.86 | C |
| ATOM | 780 | C   | GLN | A | 112 | 22.790 | 36.598 | 51.948 | 1.00 | 44.00 | C |
| ATOM | 781 | O   | GLN | A | 112 | 21.774 | 35.994 | 52.280 | 1.00 | 44.39 | O |
| ATOM | 782 | CB  | GLN | A | 112 | 24.535 | 36.428 | 53.706 | 1.00 | 44.29 | C |
| ATOM | 783 | CG  | GLN | A | 112 | 25.923 | 35.985 | 54.166 | 1.00 | 46.45 | C |



|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 784 | CD  | GLN | A | 112 | 26.050 | 34.477 | 54.296 | 1.00 | 49.14 | C |
| ATOM | 785 | OE1 | GLN | A | 112 | 25.523 | 33.733 | 53.466 | 1.00 | 50.83 | O |
| ATOM | 786 | NE2 | GLN | A | 112 | 26.756 | 34.022 | 55.332 | 1.00 | 50.52 | N |
| ATOM | 787 | N   | ASN | A | 113 | 22.765 | 37.759 | 51.299 | 1.00 | 43.96 | N |
| ATOM | 788 | CA  | ASN | A | 113 | 21.504 | 38.416 | 50.971 | 1.00 | 44.15 | C |
| ATOM | 789 | C   | ASN | A | 113 | 20.827 | 37.921 | 49.679 | 1.00 | 44.12 | C |
| ATOM | 790 | O   | ASN | A | 113 | 19.768 | 38.431 | 49.309 | 1.00 | 44.11 | O |
| ATOM | 791 | CB  | ASN | A | 113 | 21.696 | 39.941 | 50.918 | 1.00 | 44.21 | C |
| ATOM | 792 | CG  | ASN | A | 113 | 22.084 | 40.541 | 52.283 | 1.00 | 44.80 | C |
| ATOM | 793 | OD1 | ASN | A | 113 | 21.759 | 39.991 | 53.349 | 1.00 | 43.65 | O |
| ATOM | 794 | ND2 | ASN | A | 113 | 22.778 | 41.675 | 52.246 | 1.00 | 44.92 | N |
| ATOM | 795 | N   | PHE | A | 114 | 21.415 | 36.939 | 48.995 | 1.00 | 43.98 | N |
| ATOM | 796 | CA  | PHE | A | 114 | 20.793 | 36.411 | 47.787 | 1.00 | 43.71 | C |
| ATOM | 797 | C   | PHE | A | 114 | 19.778 | 35.345 | 48.150 | 1.00 | 43.76 | C |
| ATOM | 798 | O   | PHE | A | 114 | 20.111 | 34.362 | 48.815 | 1.00 | 43.32 | O |
| ATOM | 799 | CB  | PHE | A | 114 | 21.813 | 35.808 | 46.833 | 1.00 | 43.82 | C |
| ATOM | 800 | CG  | PHE | A | 114 | 21.184 | 35.128 | 45.650 | 1.00 | 43.80 | C |
| ATOM | 801 | CD1 | PHE | A | 114 | 20.567 | 35.881 | 44.661 | 1.00 | 43.54 | C |
| ATOM | 802 | CD2 | PHE | A | 114 | 21.170 | 33.745 | 45.541 | 1.00 | 43.65 | C |
| ATOM | 803 | CE1 | PHE | A | 114 | 19.963 | 35.276 | 43.587 | 1.00 | 43.55 | C |
| ATOM | 804 | CE2 | PHE | A | 114 | 20.566 | 33.129 | 44.451 | 1.00 | 43.21 | C |
| ATOM | 805 | CZ  | PHE | A | 114 | 19.961 | 33.897 | 43.476 | 1.00 | 42.89 | C |
| ATOM | 806 | N   | LYS | A | 115 | 18.543 | 35.543 | 47.705 | 1.00 | 43.96 | N |
| ATOM | 807 | CA  | LYS | A | 115 | 17.459 | 34.613 | 47.999 | 1.00 | 44.38 | C |
| ATOM | 808 | C   | LYS | A | 115 | 16.933 | 34.026 | 46.693 | 1.00 | 44.04 | C |
| ATOM | 809 | O   | LYS | A | 115 | 16.213 | 34.687 | 45.945 | 1.00 | 43.97 | O |
| ATOM | 810 | CB  | LYS | A | 115 | 16.342 | 35.329 | 48.761 | 1.00 | 44.79 | C |
| ATOM | 811 | CG  | LYS | A | 115 | 16.763 | 35.866 | 50.129 | 1.00 | 46.74 | C |
| ATOM | 812 | CD  | LYS | A | 115 | 17.021 | 34.744 | 51.130 | 1.00 | 48.83 | C |
| ATOM | 813 | CE  | LYS | A | 115 | 17.461 | 35.288 | 52.484 | 1.00 | 50.18 | C |
| ATOM | 814 | NZ  | LYS | A | 115 | 17.498 | 34.224 | 53.539 | 1.00 | 51.05 | N |
| ATOM | 815 | N   | PRO | A | 116 | 17.270 | 32.771 | 46.433 | 1.00 | 43.65 | N |
| ATOM | 816 | CA  | PRO | A | 116 | 16.918 | 32.133 | 45.160 | 1.00 | 43.43 | C |
| ATOM | 817 | C   | PRO | A | 116 | 15.415 | 32.034 | 44.969 | 1.00 | 42.76 | C |
| ATOM | 818 | O   | PRO | A | 116 | 14.711 | 31.724 | 45.915 | 1.00 | 42.78 | O |
| ATOM | 819 | CB  | PRO | A | 116 | 17.525 | 30.732 | 45.273 | 1.00 | 43.57 | C |
| ATOM | 820 | CG  | PRO | A | 116 | 18.385 | 30.743 | 46.496 | 1.00 | 43.88 | C |
| ATOM | 821 | CD  | PRO | A | 116 | 17.948 | 31.855 | 47.359 | 1.00 | 43.68 | C |
| ATOM | 822 | N   | ARG | A | 117 | 14.940 | 32.306 | 43.761 | 1.00 | 42.20 | N |
| ATOM | 823 | CA  | ARG | A | 117 | 13.518 | 32.214 | 43.451 | 1.00 | 41.56 | C |
| ATOM | 824 | C   | ARG | A | 117 | 13.140 | 30.780 | 43.104 | 1.00 | 41.00 | C |
| ATOM | 825 | O   | ARG | A | 117 | 11.957 | 30.461 | 43.007 | 1.00 | 41.15 | O |
| ATOM | 826 | CB  | ARG | A | 117 | 13.164 | 33.132 | 42.311 | 1.00 | 41.47 | C |
| ATOM | 827 | N   | SER | A | 118 | 14.139 | 29.925 | 42.904 | 1.00 | 40.00 | N |
| ATOM | 828 | CA  | SER | A | 118 | 13.882 | 28.517 | 42.654 | 1.00 | 39.60 | C |
| ATOM | 829 | C   | SER | A | 118 | 14.700 | 27.655 | 43.621 | 1.00 | 39.30 | C |
| ATOM | 830 | O   | SER | A | 118 | 15.756 | 28.078 | 44.087 | 1.00 | 39.24 | O |
| ATOM | 831 | CB  | SER | A | 118 | 14.184 | 28.158 | 41.196 | 1.00 | 39.30 | C |
| ATOM | 832 | OG  | SER | A | 118 | 15.560 | 28.228 | 40.942 | 1.00 | 38.53 | O |
| ATOM | 833 | N   | ASN | A | 119 | 14.180 | 26.471 | 43.943 | 1.00 | 38.96 | N |
| ATOM | 834 | CA  | ASN | A | 119 | 14.838 | 25.537 | 44.854 | 1.00 | 38.95 | C |
| ATOM | 835 | C   | ASN | A | 119 | 15.115 | 24.215 | 44.160 | 1.00 | 37.99 | C |
| ATOM | 836 | O   | ASN | A | 119 | 14.314 | 23.751 | 43.359 | 1.00 | 37.35 | O |
| ATOM | 837 | CB  | ASN | A | 119 | 13.958 | 25.220 | 46.068 | 1.00 | 39.54 | C |
| ATOM | 838 | CG  | ASN | A | 119 | 13.466 | 26.456 | 46.797 | 1.00 | 41.82 | C |
| ATOM | 839 | OD1 | ASN | A | 119 | 14.255 | 27.279 | 47.289 | 1.00 | 44.50 | O |
| ATOM | 840 | ND2 | ASN | A | 119 | 12.145 | 26.574 | 46.906 | 1.00 | 44.99 | N |
| ATOM | 841 | N   | ARG | A | 120 | 16.243 | 23.607 | 44.492 | 1.00 | 37.46 | N |
| ATOM | 842 | CA  | ARG | A | 120 | 16.627 | 22.325 | 43.927 | 1.00 | 37.15 | C |
| ATOM | 843 | C   | ARG | A | 120 | 16.209 | 21.193 | 44.844 | 1.00 | 37.03 | C |
| ATOM | 844 | O   | ARG | A | 120 | 16.359 | 21.272 | 46.069 | 1.00 | 37.28 | O |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 845 | CB  | ARG | A | 120 | 18.144 | 22.264 | 43.730 | 1.00 | 37.07 | C |
| ATOM | 846 | CG  | ARG | A | 120 | 18.632 | 21.020 | 42.993 | 1.00 | 36.32 | C |
| ATOM | 847 | CD  | ARG | A | 120 | 20.152 | 20.886 | 42.938 | 1.00 | 35.46 | C |
| ATOM | 848 | NE  | ARG | A | 120 | 20.777 | 21.277 | 44.198 | 1.00 | 34.29 | N |
| ATOM | 849 | CZ  | ARG | A | 120 | 21.049 | 20.445 | 45.202 | 1.00 | 36.66 | C |
| ATOM | 850 | NH1 | ARG | A | 120 | 20.753 | 19.147 | 45.122 | 1.00 | 35.60 | N |
| ATOM | 851 | NH2 | ARG | A | 120 | 21.614 | 20.915 | 46.305 | 1.00 | 37.13 | N |
| ATOM | 852 | N   | GLU | A | 121 | 15.665 | 20.141 | 44.250 | 1.00 | 36.76 | N |
| ATOM | 853 | CA  | GLU | A | 121 | 15.326 | 18.944 | 44.993 | 1.00 | 36.29 | C |
| ATOM | 854 | C   | GLU | A | 121 | 15.810 | 17.746 | 44.187 | 1.00 | 35.35 | C |
| ATOM | 855 | O   | GLU | A | 121 | 15.709 | 17.726 | 42.953 | 1.00 | 35.38 | O |
| ATOM | 856 | CB  | GLU | A | 121 | 13.820 | 18.863 | 45.262 | 1.00 | 36.78 | C |
| ATOM | 857 | CG  | GLU | A | 121 | 13.398 | 17.585 | 45.971 | 1.00 | 39.29 | C |
| ATOM | 858 | CD  | GLU | A | 121 | 12.126 | 17.732 | 46.795 | 1.00 | 42.09 | C |
| ATOM | 859 | OE1 | GLU | A | 121 | 12.200 | 18.310 | 47.904 | 1.00 | 45.56 | O |
| ATOM | 860 | OE2 | GLU | A | 121 | 11.059 | 17.254 | 46.350 | 1.00 | 43.04 | O |
| ATOM | 861 | N   | GLU | A | 122 | 16.366 | 16.764 | 44.886 | 1.00 | 34.04 | N |
| ATOM | 862 | CA  | GLU | A | 122 | 16.840 | 15.547 | 44.266 | 1.00 | 33.04 | C |
| ATOM | 863 | C   | GLU | A | 122 | 15.748 | 14.518 | 44.415 | 1.00 | 32.55 | C |
| ATOM | 864 | O   | GLU | A | 122 | 15.253 | 14.306 | 45.511 | 1.00 | 32.52 | O |
| ATOM | 865 | CB  | GLU | A | 122 | 18.103 | 15.052 | 44.961 | 1.00 | 32.71 | C |
| ATOM | 866 | CG  | GLU | A | 122 | 19.265 | 16.018 | 44.885 | 1.00 | 31.86 | C |
| ATOM | 867 | CD  | GLU | A | 122 | 19.705 | 16.296 | 43.454 | 1.00 | 31.04 | C |
| ATOM | 868 | OE1 | GLU | A | 122 | 20.065 | 15.331 | 42.757 | 1.00 | 29.68 | O |
| ATOM | 869 | OE2 | GLU | A | 122 | 19.694 | 17.479 | 43.025 | 1.00 | 29.20 | O |
| ATOM | 870 | N   | MET | A | 123 | 15.349 | 13.885 | 43.321 | 1.00 | 31.83 | N |
| ATOM | 871 | CA  | MET | A | 123 | 14.329 | 12.858 | 43.415 | 1.00 | 31.40 | C |
| ATOM | 872 | C   | MET | A | 123 | 14.532 | 11.820 | 42.343 | 1.00 | 30.68 | C |
| ATOM | 873 | O   | MET | A | 123 | 15.380 | 11.982 | 41.457 | 1.00 | 30.07 | O |
| ATOM | 874 | CB  | MET | A | 123 | 12.931 | 13.466 | 43.309 | 1.00 | 31.52 | C |
| ATOM | 875 | CG  | MET | A | 123 | 12.667 | 14.205 | 42.032 | 1.00 | 32.93 | C |
| ATOM | 876 | SD  | MET | A | 123 | 11.115 | 15.145 | 42.034 | 1.00 | 35.27 | S |
| ATOM | 877 | CE  | MET | A | 123 | 11.554 | 16.565 | 42.966 | 1.00 | 35.33 | C |
| ATOM | 878 | N   | LYS | A | 124 | 13.766 | 10.738 | 42.464 | 1.00 | 29.85 | N |
| ATOM | 879 | CA  | LYS | A | 124 | 13.752 | 9.671  | 41.483 | 1.00 | 29.22 | C |
| ATOM | 880 | C   | LYS | A | 124 | 12.891 | 10.140 | 40.307 | 1.00 | 28.45 | C |
| ATOM | 881 | O   | LYS | A | 124 | 12.066 | 11.039 | 40.466 | 1.00 | 27.39 | O |
| ATOM | 882 | CB  | LYS | A | 124 | 13.183 | 8.389  | 42.100 | 1.00 | 29.57 | C |
| ATOM | 883 | CG  | LYS | A | 124 | 13.954 | 7.857  | 43.321 | 1.00 | 29.88 | C |
| ATOM | 884 | CD  | LYS | A | 124 | 15.392 | 7.501  | 42.950 | 1.00 | 30.48 | C |
| ATOM | 885 | CE  | LYS | A | 124 | 16.231 | 7.129  | 44.167 | 1.00 | 30.33 | C |
| ATOM | 886 | NZ  | LYS | A | 124 | 17.691 | 7.276  | 43.872 | 1.00 | 30.47 | N |
| ATOM | 887 | N   | PHE | A | 125 | 13.075 | 9.536  | 39.133 | 1.00 | 27.71 | N |
| ATOM | 888 | CA  | PHE | A | 125 | 12.364 | 10.000 | 37.949 | 1.00 | 27.22 | C |
| ATOM | 889 | C   | PHE | A | 125 | 10.869 | 9.891  | 38.114 | 1.00 | 27.29 | C |
| ATOM | 890 | O   | PHE | A | 125 | 10.138 | 10.825 | 37.801 | 1.00 | 26.75 | O |
| ATOM | 891 | CB  | PHE | A | 125 | 12.794 | 9.270  | 36.681 | 1.00 | 26.90 | C |
| ATOM | 892 | CG  | PHE | A | 125 | 12.494 | 10.051 | 35.433 | 1.00 | 27.63 | C |
| ATOM | 893 | CD1 | PHE | A | 125 | 13.330 | 11.083 | 35.032 | 1.00 | 27.70 | C |
| ATOM | 894 | CD2 | PHE | A | 125 | 11.351 | 9.802  | 34.702 | 1.00 | 28.29 | C |
| ATOM | 895 | CE1 | PHE | A | 125 | 13.059 | 11.828 | 33.905 | 1.00 | 27.96 | C |
| ATOM | 896 | CE2 | PHE | A | 125 | 11.065 | 10.540 | 33.563 | 1.00 | 29.16 | C |
| ATOM | 897 | CZ  | PHE | A | 125 | 11.924 | 11.568 | 33.167 | 1.00 | 28.71 | C |
| ATOM | 898 | N   | HIS | A | 126 | 10.426 | 8.743  | 38.620 | 1.00 | 27.46 | N |
| ATOM | 899 | CA  | HIS | A | 126 | 9.013  | 8.499  | 38.832 | 1.00 | 27.77 | C |
| ATOM | 900 | C   | HIS | A | 126 | 8.430  | 9.522  | 39.794 | 1.00 | 27.71 | C |
| ATOM | 901 | O   | HIS | A | 126 | 7.245  | 9.821  | 39.731 | 1.00 | 27.27 | O |
| ATOM | 902 | CB  | HIS | A | 126 | 8.770  | 7.056  | 39.329 | 1.00 | 27.96 | C |
| ATOM | 903 | CG  | HIS | A | 126 | 8.897  | 6.880  | 40.812 | 1.00 | 28.47 | C |
| ATOM | 904 | ND1 | HIS | A | 126 | 7.831  | 7.026  | 41.672 | 1.00 | 29.29 | N |
| ATOM | 905 | CD2 | HIS | A | 126 | 9.961  | 6.552  | 41.585 | 1.00 | 29.43 | C |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 906 | CE1 | HIS | A | 126 | 8.236  | 6.812  | 42.912 | 1.00 | 30.26 | C |
| ATOM | 907 | NE2 | HIS | A | 126 | 9.525  | 6.524  | 42.887 | 1.00 | 29.64 | N |
| ATOM | 908 | N   | GLU | A | 127 | 9.262  | 10.059 | 40.679 | 1.00 | 28.09 | N |
| ATOM | 909 | CA  | GLU | A | 127 | 8.803  | 11.078 | 41.615 | 1.00 | 28.68 | C |
| ATOM | 910 | C   | GLU | A | 127 | 8.585  | 12.400 | 40.865 | 1.00 | 28.99 | C |
| ATOM | 911 | O   | GLU | A | 127 | 7.626  | 13.129 | 41.123 | 1.00 | 29.15 | O |
| ATOM | 912 | CB  | GLU | A | 127 | 9.795  | 11.233 | 42.775 | 1.00 | 28.52 | C |
| ATOM | 913 | CG  | GLU | A | 127 | 9.931  | 9.968  | 43.626 | 1.00 | 29.84 | C |
| ATOM | 914 | CD  | GLU | A | 127 | 10.873 | 10.121 | 44.810 | 1.00 | 30.26 | C |
| ATOM | 915 | OE1 | GLU | A | 127 | 12.069 | 10.398 | 44.603 | 1.00 | 29.68 | O |
| ATOM | 916 | OE2 | GLU | A | 127 | 10.410 | 9.943  | 45.962 | 1.00 | 32.95 | O |
| ATOM | 917 | N   | PHE | A | 128 | 9.471  | 12.696 | 39.927 | 1.00 | 29.39 | N |
| ATOM | 918 | CA  | PHE | A | 128 | 9.354  | 13.914 | 39.119 | 1.00 | 29.64 | C |
| ATOM | 919 | C   | PHE | A | 128 | 8.047  | 13.859 | 38.333 | 1.00 | 30.31 | C |
| ATOM | 920 | O   | PHE | A | 128 | 7.274  | 14.817 | 38.294 | 1.00 | 29.97 | O |
| ATOM | 921 | CB  | PHE | A | 128 | 10.551 | 14.017 | 38.167 | 1.00 | 29.10 | C |
| ATOM | 922 | CG  | PHE | A | 128 | 10.337 | 14.950 | 36.991 | 1.00 | 28.33 | C |
| ATOM | 923 | CD1 | PHE | A | 128 | 10.106 | 16.301 | 37.188 | 1.00 | 26.53 | C |
| ATOM | 924 | CD2 | PHE | A | 128 | 10.397 | 14.475 | 35.696 | 1.00 | 26.99 | C |
| ATOM | 925 | CE1 | PHE | A | 128 | 9.920  | 17.149 | 36.120 | 1.00 | 27.50 | C |
| ATOM | 926 | CE2 | PHE | A | 128 | 10.217 | 15.341 | 34.610 | 1.00 | 28.49 | C |
| ATOM | 927 | CZ  | PHE | A | 128 | 9.976  | 16.668 | 34.823 | 1.00 | 26.78 | C |
| ATOM | 928 | N   | VAL | A | 129 | 7.797  | 12.705 | 37.736 | 1.00 | 31.32 | N |
| ATOM | 929 | CA  | VAL | A | 129 | 6.603  | 12.499 | 36.930 | 1.00 | 32.38 | C |
| ATOM | 930 | C   | VAL | A | 129 | 5.338  | 12.658 | 37.775 | 1.00 | 32.96 | C |
| ATOM | 931 | O   | VAL | A | 129 | 4.398  | 13.362 | 37.388 | 1.00 | 32.79 | O |
| ATOM | 932 | CB  | VAL | A | 129 | 6.606  | 11.094 | 36.313 | 1.00 | 32.48 | C |
| ATOM | 933 | CG1 | VAL | A | 129 | 5.313  | 10.840 | 35.551 | 1.00 | 32.96 | C |
| ATOM | 934 | CG2 | VAL | A | 129 | 7.828  | 10.901 | 35.417 | 1.00 | 31.98 | C |
| ATOM | 935 | N   | GLU | A | 130 | 5.329  | 11.993 | 38.925 | 1.00 | 33.61 | N |
| ATOM | 936 | CA  | GLU | A | 130 | 4.205  | 12.067 | 39.853 | 1.00 | 34.29 | C |
| ATOM | 937 | C   | GLU | A | 130 | 3.963  | 13.515 | 40.246 | 1.00 | 34.51 | C |
| ATOM | 938 | O   | GLU | A | 130 | 2.832  | 13.986 | 40.220 | 1.00 | 33.80 | O |
| ATOM | 939 | CB  | GLU | A | 130 | 4.481  | 11.206 | 41.087 | 1.00 | 34.35 | C |
| ATOM | 940 | CG  | GLU | A | 130 | 4.372  | 9.711  | 40.815 | 1.00 | 34.92 | C |
| ATOM | 941 | CD  | GLU | A | 130 | 5.204  | 8.858  | 41.761 | 1.00 | 35.66 | C |
| ATOM | 942 | OE1 | GLU | A | 130 | 5.595  | 9.345  | 42.845 | 1.00 | 36.55 | O |
| ATOM | 943 | OE2 | GLU | A | 130 | 5.477  | 7.692  | 41.407 | 1.00 | 36.06 | O |
| ATOM | 944 | N   | LYS | A | 131 | 5.033  | 14.223 | 40.587 | 1.00 | 35.27 | N |
| ATOM | 945 | CA  | LYS | A | 131 | 4.912  | 15.632 | 40.920 | 1.00 | 36.15 | C |
| ATOM | 946 | C   | LYS | A | 131 | 4.286  | 16.408 | 39.758 | 1.00 | 36.63 | C |
| ATOM | 947 | O   | LYS | A | 131 | 3.420  | 17.253 | 39.972 | 1.00 | 36.42 | O |
| ATOM | 948 | CB  | LYS | A | 131 | 6.269  | 16.240 | 41.261 | 1.00 | 36.51 | C |
| ATOM | 949 | CG  | LYS | A | 131 | 6.467  | 16.623 | 42.712 | 1.00 | 37.67 | C |
| ATOM | 950 | CD  | LYS | A | 131 | 7.125  | 18.001 | 42.822 | 1.00 | 38.95 | C |
| ATOM | 951 | CE  | LYS | A | 131 | 7.581  | 18.324 | 44.252 | 1.00 | 40.39 | C |
| ATOM | 952 | NZ  | LYS | A | 131 | 8.073  | 19.747 | 44.404 | 1.00 | 40.82 | N |
| ATOM | 953 | N   | LEU | A | 132 | 4.725  | 16.142 | 38.532 | 1.00 | 37.30 | N |
| ATOM | 954 | CA  | LEU | A | 132 | 4.156  | 16.845 | 37.383 | 1.00 | 38.29 | C |
| ATOM | 955 | C   | LEU | A | 132 | 2.669  | 16.557 | 37.280 | 1.00 | 38.83 | C |
| ATOM | 956 | O   | LEU | A | 132 | 1.875  | 17.449 | 36.976 | 1.00 | 38.56 | O |
| ATOM | 957 | CB  | LEU | A | 132 | 4.819  | 16.424 | 36.081 | 1.00 | 38.42 | C |
| ATOM | 958 | CG  | LEU | A | 132 | 6.224  | 16.916 | 35.791 | 1.00 | 39.15 | C |
| ATOM | 959 | CD1 | LEU | A | 132 | 6.671  | 16.296 | 34.485 | 1.00 | 39.76 | C |
| ATOM | 960 | CD2 | LEU | A | 132 | 6.281  | 18.433 | 35.712 | 1.00 | 39.81 | C |
| ATOM | 961 | N   | GLN | A | 133 | 2.311  | 15.300 | 37.529 | 1.00 | 39.68 | N |
| ATOM | 962 | CA  | GLN | A | 133 | 0.920  | 14.863 | 37.495 | 1.00 | 40.45 | C |
| ATOM | 963 | C   | GLN | A | 133 | 0.057  | 15.580 | 38.541 | 1.00 | 41.05 | C |
| ATOM | 964 | O   | GLN | A | 133 | -1.035 | 16.040 | 38.222 | 1.00 | 41.20 | O |
| ATOM | 965 | CB  | GLN | A | 133 | 0.835  | 13.344 | 37.681 | 1.00 | 40.31 | C |
| ATOM | 966 | N   | ASP | A | 134 | 0.542  | 15.682 | 39.777 | 1.00 | 41.89 | N |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 967  | CA  | ASP | A | 134 | -0.232 | 16.313 | 40.854 | 1.00 | 42.72 | C |
| ATOM | 968  | C   | ASP | A | 134 | -0.506 | 17.792 | 40.576 | 1.00 | 42.60 | C |
| ATOM | 969  | O   | ASP | A | 134 | -1.570 | 18.316 | 40.900 | 1.00 | 42.25 | O |
| ATOM | 970  | CB  | ASP | A | 134 | 0.491  | 16.169 | 42.200 | 1.00 | 43.21 | C |
| ATOM | 971  | CG  | ASP | A | 134 | -0.429 | 16.419 | 43.396 | 1.00 | 45.71 | C |
| ATOM | 972  | OD1 | ASP | A | 134 | -1.566 | 16.916 | 43.213 | 1.00 | 48.39 | O |
| ATOM | 973  | OD2 | ASP | A | 134 | -0.104 | 16.131 | 44.571 | 1.00 | 49.60 | O |
| ATOM | 974  | N   | ILE | A | 135 | 0.467  | 18.467 | 39.981 | 1.00 | 42.77 | N |
| ATOM | 975  | CA  | ILE | A | 135 | 0.306  | 19.872 | 39.660 | 1.00 | 42.91 | C |
| ATOM | 976  | C   | ILE | A | 135 | -0.793 | 20.050 | 38.626 | 1.00 | 43.15 | C |
| ATOM | 977  | O   | ILE | A | 135 | -1.690 | 20.871 | 38.800 | 1.00 | 43.03 | O |
| ATOM | 978  | CB  | ILE | A | 135 | 1.623  | 20.443 | 39.155 | 1.00 | 42.94 | C |
| ATOM | 979  | CG1 | ILE | A | 135 | 2.586  | 20.607 | 40.330 | 1.00 | 43.10 | C |
| ATOM | 980  | CG2 | ILE | A | 135 | 1.396  | 21.778 | 38.473 | 1.00 | 42.80 | C |
| ATOM | 981  | CD1 | ILE | A | 135 | 4.040  | 20.621 | 39.934 | 1.00 | 43.49 | C |
| ATOM | 982  | N   | GLN | A | 136 | -0.716 | 19.272 | 37.554 | 1.00 | 43.64 | N |
| ATOM | 983  | CA  | GLN | A | 136 | -1.712 | 19.321 | 36.496 | 1.00 | 44.17 | C |
| ATOM | 984  | C   | GLN | A | 136 | -3.103 | 19.129 | 37.081 | 1.00 | 44.65 | C |
| ATOM | 985  | O   | GLN | A | 136 | -3.976 | 19.984 | 36.936 | 1.00 | 44.71 | O |
| ATOM | 986  | CB  | GLN | A | 136 | -1.431 | 18.240 | 35.466 | 1.00 | 44.19 | C |
| ATOM | 987  | N   | GLN | A | 137 | -3.289 | 18.014 | 37.776 | 1.00 | 45.23 | N |
| ATOM | 988  | CA  | GLN | A | 137 | -4.596 | 17.654 | 38.314 | 1.00 | 45.66 | C |
| ATOM | 989  | C   | GLN | A | 137 | -5.146 | 18.696 | 39.277 | 1.00 | 45.88 | C |
| ATOM | 990  | O   | GLN | A | 137 | -6.337 | 19.005 | 39.238 | 1.00 | 46.33 | O |
| ATOM | 991  | CB  | GLN | A | 137 | -4.535 | 16.277 | 38.991 | 1.00 | 45.74 | C |
| ATOM | 992  | N   | ARG | A | 138 | -4.288 | 19.246 | 40.131 | 1.00 | 45.93 | N |
| ATOM | 993  | CA  | ARG | A | 138 | -4.740 | 20.211 | 41.132 | 1.00 | 45.84 | C |
| ATOM | 994  | C   | ARG | A | 138 | -4.720 | 21.640 | 40.592 | 1.00 | 45.53 | C |
| ATOM | 995  | O   | ARG | A | 138 | -4.911 | 22.598 | 41.344 | 1.00 | 45.72 | O |
| ATOM | 996  | CB  | ARG | A | 138 | -3.880 | 20.108 | 42.398 | 1.00 | 45.92 | C |
| ATOM | 997  | CG  | ARG | A | 138 | -2.551 | 20.866 | 42.340 | 1.00 | 46.84 | C |
| ATOM | 998  | CD  | ARG | A | 138 | -1.589 | 20.458 | 43.437 | 1.00 | 47.70 | C |
| ATOM | 999  | NE  | ARG | A | 138 | -0.509 | 21.418 | 43.652 | 1.00 | 47.78 | N |
| ATOM | 1000 | CZ  | ARG | A | 138 | 0.788  | 21.125 | 43.578 | 1.00 | 49.17 | C |
| ATOM | 1001 | NH1 | ARG | A | 138 | 1.186  | 19.897 | 43.274 | 1.00 | 50.12 | N |
| ATOM | 1002 | NH2 | ARG | A | 138 | 1.702  | 22.064 | 43.798 | 1.00 | 49.52 | N |
| ATOM | 1003 | N   | GLY | A | 139 | -4.492 | 21.783 | 39.290 | 1.00 | 44.99 | N |
| ATOM | 1004 | CA  | GLY | A | 139 | -4.419 | 23.094 | 38.669 | 1.00 | 44.52 | C |
| ATOM | 1005 | C   | GLY | A | 139 | -3.412 | 24.041 | 39.310 | 1.00 | 44.06 | C |
| ATOM | 1006 | O   | GLY | A | 139 | -3.551 | 25.259 | 39.203 | 1.00 | 44.28 | O |
| ATOM | 1007 | N   | GLY | A | 140 | -2.382 | 23.495 | 39.953 | 1.00 | 43.28 | N |
| ATOM | 1008 | CA  | GLY | A | 140 | -1.388 | 24.309 | 40.629 | 1.00 | 42.49 | C |
| ATOM | 1009 | C   | GLY | A | 140 | -0.609 | 25.218 | 39.694 | 1.00 | 41.92 | C |
| ATOM | 1010 | O   | GLY | A | 140 | -0.556 | 24.989 | 38.480 | 1.00 | 41.85 | O |
| ATOM | 1011 | N   | GLU | A | 141 | -0.004 | 26.264 | 40.250 | 1.00 | 40.90 | N |
| ATOM | 1012 | CA  | GLU | A | 141 | 0.789  | 27.186 | 39.444 | 1.00 | 40.07 | C |
| ATOM | 1013 | C   | GLU | A | 141 | 2.286  | 26.884 | 39.549 | 1.00 | 38.68 | C |
| ATOM | 1014 | O   | GLU | A | 141 | 3.096  | 27.503 | 38.867 | 1.00 | 38.67 | O |
| ATOM | 1015 | CB  | GLU | A | 141 | 0.513  | 28.644 | 39.839 | 1.00 | 40.36 | C |
| ATOM | 1016 | CG  | GLU | A | 141 | -0.799 | 29.224 | 39.309 | 1.00 | 41.91 | C |
| ATOM | 1017 | CD  | GLU | A | 141 | -1.001 | 29.042 | 37.805 | 1.00 | 44.25 | C |
| ATOM | 1018 | OE1 | GLU | A | 141 | 0.004  | 29.008 | 37.043 | 1.00 | 45.69 | O |
| ATOM | 1019 | OE2 | GLU | A | 141 | -2.181 | 28.940 | 37.380 | 1.00 | 44.55 | O |
| ATOM | 1020 | N   | GLU | A | 142 | 2.648  | 25.944 | 40.413 | 1.00 | 37.02 | N |
| ATOM | 1021 | CA  | GLU | A | 142 | 4.040  | 25.573 | 40.596 | 1.00 | 35.61 | C |
| ATOM | 1022 | C   | GLU | A | 142 | 4.629  | 25.120 | 39.265 | 1.00 | 34.41 | C |
| ATOM | 1023 | O   | GLU | A | 142 | 3.923  | 24.594 | 38.408 | 1.00 | 34.25 | O |
| ATOM | 1024 | CB  | GLU | A | 142 | 4.150  | 24.443 | 41.627 | 1.00 | 35.49 | C |
| ATOM | 1025 | CG  | GLU | A | 142 | 5.571  | 24.173 | 42.095 | 1.00 | 35.47 | C |
| ATOM | 1026 | CD  | GLU | A | 142 | 5.710  | 22.944 | 42.978 | 1.00 | 36.48 | C |
| ATOM | 1027 | OE1 | GLU | A | 142 | 4.733  | 22.174 | 43.142 | 1.00 | 37.45 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1028 | OE2 | GLU | A | 142 | 6.821  | 22.739 | 43.511 | 1.00 | 36.76 | O |
| ATOM | 1029 | N   | ARG | A | 143 | 5.926  | 25.323 | 39.096 | 1.00 | 32.91 | N |
| ATOM | 1030 | CA  | ARG | A | 143 | 6.596  | 24.893 | 37.884 | 1.00 | 31.95 | C |
| ATOM | 1031 | C   | ARG | A | 143 | 7.803  | 24.058 | 38.214 | 1.00 | 30.62 | C |
| ATOM | 1032 | O   | ARG | A | 143 | 8.514  | 24.354 | 39.166 | 1.00 | 30.75 | O |
| ATOM | 1033 | CB  | ARG | A | 143 | 7.072  | 26.097 | 37.082 | 1.00 | 32.19 | C |
| ATOM | 1034 | CG  | ARG | A | 143 | 5.968  | 26.912 | 36.447 | 1.00 | 32.57 | C |
| ATOM | 1035 | CD  | ARG | A | 143 | 6.507  | 28.170 | 35.801 | 1.00 | 32.53 | C |
| ATOM | 1036 | NE  | ARG | A | 143 | 5.492  | 28.885 | 35.037 | 1.00 | 32.25 | N |
| ATOM | 1037 | CZ  | ARG | A | 143 | 5.158  | 28.617 | 33.790 | 1.00 | 31.80 | C |
| ATOM | 1038 | NH1 | ARG | A | 143 | 5.757  | 27.637 | 33.105 | 1.00 | 31.28 | N |
| ATOM | 1039 | NH2 | ARG | A | 143 | 4.214  | 29.345 | 33.221 | 1.00 | 32.77 | N |
| ATOM | 1040 | N   | LEU | A | 144 | 8.054  | 23.028 | 37.417 | 1.00 | 28.97 | N |
| ATOM | 1041 | CA  | LEU | A | 144 | 9.235  | 22.219 | 37.617 | 1.00 | 28.09 | C |
| ATOM | 1042 | C   | LEU | A | 144 | 10.150 | 22.257 | 36.398 | 1.00 | 27.14 | C |
| ATOM | 1043 | O   | LEU | A | 144 | 9.690  | 22.418 | 35.272 | 1.00 | 26.74 | O |
| ATOM | 1044 | CB  | LEU | A | 144 | 8.834  | 20.783 | 37.887 | 1.00 | 28.28 | C |
| ATOM | 1045 | CG  | LEU | A | 144 | 7.839  | 20.606 | 39.038 | 1.00 | 28.89 | C |
| ATOM | 1046 | CD1 | LEU | A | 144 | 7.515  | 19.123 | 39.216 | 1.00 | 29.62 | C |
| ATOM | 1047 | CD2 | LEU | A | 144 | 8.364  | 21.212 | 40.333 | 1.00 | 27.84 | C |
| ATOM | 1048 | N   | TYR | A | 145 | 11.447 | 22.102 | 36.636 | 1.00 | 25.69 | N |
| ATOM | 1049 | CA  | TYR | A | 145 | 12.395 | 21.976 | 35.548 | 1.00 | 25.05 | C |
| ATOM | 1050 | C   | TYR | A | 145 | 13.459 | 20.957 | 35.968 | 1.00 | 25.00 | C |
| ATOM | 1051 | O   | TYR | A | 145 | 14.239 | 21.193 | 36.881 | 1.00 | 25.01 | O |
| ATOM | 1052 | CB  | TYR | A | 145 | 13.022 | 23.327 | 35.183 | 1.00 | 24.76 | C |
| ATOM | 1053 | CG  | TYR | A | 145 | 13.471 | 23.485 | 33.728 | 1.00 | 23.25 | C |
| ATOM | 1054 | CD1 | TYR | A | 145 | 13.739 | 22.385 | 32.931 | 1.00 | 21.70 | C |
| ATOM | 1055 | CD2 | TYR | A | 145 | 13.667 | 24.746 | 33.175 | 1.00 | 22.16 | C |
| ATOM | 1056 | CE1 | TYR | A | 145 | 14.154 | 22.526 | 31.620 | 1.00 | 20.98 | C |
| ATOM | 1057 | CE2 | TYR | A | 145 | 14.097 | 24.904 | 31.846 | 1.00 | 21.30 | C |
| ATOM | 1058 | CZ  | TYR | A | 145 | 14.332 | 23.799 | 31.071 | 1.00 | 20.66 | C |
| ATOM | 1059 | OH  | TYR | A | 145 | 14.737 | 23.933 | 29.740 | 1.00 | 18.41 | O |
| ATOM | 1060 | N   | LEU | A | 146 | 13.446 | 19.808 | 35.318 | 1.00 | 24.95 | N |
| ATOM | 1061 | CA  | LEU | A | 146 | 14.453 | 18.787 | 35.547 | 1.00 | 25.43 | C |
| ATOM | 1062 | C   | LEU | A | 146 | 15.678 | 19.100 | 34.694 | 1.00 | 24.91 | C |
| ATOM | 1063 | O   | LEU | A | 146 | 15.555 | 19.313 | 33.493 | 1.00 | 24.10 | O |
| ATOM | 1064 | CB  | LEU | A | 146 | 13.907 | 17.419 | 35.162 | 1.00 | 25.59 | C |
| ATOM | 1065 | CG  | LEU | A | 146 | 14.875 | 16.238 | 35.334 | 1.00 | 27.52 | C |
| ATOM | 1066 | CD1 | LEU | A | 146 | 14.111 | 14.966 | 35.672 | 1.00 | 26.95 | C |
| ATOM | 1067 | CD2 | LEU | A | 146 | 15.742 | 16.023 | 34.084 | 1.00 | 29.46 | C |
| ATOM | 1068 | N   | GLN | A | 147 | 16.845 | 19.097 | 35.330 | 1.00 | 24.91 | N |
| ATOM | 1069 | CA  | GLN | A | 147 | 18.115 | 19.394 | 34.685 | 1.00 | 25.27 | C |
| ATOM | 1070 | C   | GLN | A | 147 | 19.146 | 18.490 | 35.317 | 1.00 | 25.28 | C |
| ATOM | 1071 | O   | GLN | A | 147 | 19.610 | 18.740 | 36.419 | 1.00 | 27.14 | O |
| ATOM | 1072 | CB  | GLN | A | 147 | 18.475 | 20.876 | 34.863 | 1.00 | 25.02 | C |
| ATOM | 1073 | CG  | GLN | A | 147 | 17.321 | 21.804 | 34.485 | 1.00 | 24.97 | C |
| ATOM | 1074 | CD  | GLN | A | 147 | 17.682 | 23.283 | 34.560 | 1.00 | 27.08 | C |
| ATOM | 1075 | OE1 | GLN | A | 147 | 16.891 | 24.149 | 34.141 | 1.00 | 27.93 | O |
| ATOM | 1076 | NE2 | GLN | A | 147 | 18.860 | 23.575 | 35.064 | 1.00 | 23.50 | N |
| ATOM | 1077 | N   | GLN | A | 148 | 19.487 | 17.428 | 34.611 | 1.00 | 25.47 | N |
| ATOM | 1078 | CA  | GLN | A | 148 | 20.319 | 16.365 | 35.146 | 1.00 | 25.45 | C |
| ATOM | 1079 | C   | GLN | A | 148 | 21.254 | 15.816 | 34.105 | 1.00 | 25.50 | C |
| ATOM | 1080 | O   | GLN | A | 148 | 20.862 | 15.485 | 32.992 | 1.00 | 25.04 | O |
| ATOM | 1081 | CB  | GLN | A | 148 | 19.436 | 15.231 | 35.640 | 1.00 | 25.37 | C |
| ATOM | 1082 | CG  | GLN | A | 148 | 20.201 | 14.021 | 36.167 | 1.00 | 26.15 | C |
| ATOM | 1083 | CD  | GLN | A | 148 | 21.129 | 14.383 | 37.314 | 1.00 | 26.56 | C |
| ATOM | 1084 | OE1 | GLN | A | 148 | 20.718 | 15.093 | 38.240 | 1.00 | 23.94 | O |
| ATOM | 1085 | NE2 | GLN | A | 148 | 22.383 | 13.916 | 37.248 | 1.00 | 25.29 | N |
| ATOM | 1086 | N   | THR | A | 149 | 22.510 | 15.769 | 34.482 | 1.00 | 25.86 | N |
| ATOM | 1087 | CA  | THR | A | 149 | 23.552 | 15.219 | 33.667 | 1.00 | 27.04 | C |
| ATOM | 1088 | C   | THR | A | 149 | 23.298 | 13.720 | 33.527 | 1.00 | 27.25 | C |

|      |      |     |           |        |        |        |      |       |   |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 1089 | O   | THR A 149 | 23.012 | 13.044 | 34.508 | 1.00 | 26.86 | O |
| ATOM | 1090 | CB  | THR A 149 | 24.903 | 15.540 | 34.375 | 1.00 | 27.42 | C |
| ATOM | 1091 | OG1 | THR A 149 | 25.300 | 16.882 | 34.020 | 1.00 | 29.80 | O |
| ATOM | 1092 | CG2 | THR A 149 | 26.034 | 14.702 | 33.873 | 1.00 | 28.98 | C |
| ATOM | 1093 | N   | LEU A 150 | 23.338 | 13.224 | 32.298 | 1.00 | 27.70 | N |
| ATOM | 1094 | CA  | LEU A 150 | 23.195 | 11.812 | 32.027 | 1.00 | 28.46 | C |
| ATOM | 1095 | C   | LEU A 150 | 24.429 | 11.076 | 32.573 | 1.00 | 28.97 | C |
| ATOM | 1096 | O   | LEU A 150 | 25.548 | 11.468 | 32.268 | 1.00 | 29.00 | O |
| ATOM | 1097 | CB  | LEU A 150 | 23.084 | 11.580 | 30.524 | 1.00 | 28.34 | C |
| ATOM | 1098 | CG  | LEU A 150 | 21.780 | 11.981 | 29.837 | 1.00 | 29.63 | C |
| ATOM | 1099 | CD1 | LEU A 150 | 21.944 | 11.862 | 28.328 | 1.00 | 30.03 | C |
| ATOM | 1100 | CD2 | LEU A 150 | 20.619 | 11.140 | 30.310 | 1.00 | 31.15 | C |
| ATOM | 1101 | N   | ASN A 151 | 24.230 | 10.030 | 33.378 | 1.00 | 29.35 | N |
| ATOM | 1102 | CA  | ASN A 151 | 25.348 | 9.258  | 33.949 | 1.00 | 29.51 | C |
| ATOM | 1103 | C   | ASN A 151 | 25.137 | 7.732  | 33.934 | 1.00 | 29.92 | C |
| ATOM | 1104 | O   | ASN A 151 | 24.162 | 7.241  | 33.348 | 1.00 | 29.73 | O |
| ATOM | 1105 | CB  | ASN A 151 | 25.590 | 9.710  | 35.385 | 1.00 | 29.78 | C |
| ATOM | 1106 | CG  | ASN A 151 | 24.362 | 9.553  | 36.241 | 1.00 | 29.19 | C |
| ATOM | 1107 | OD1 | ASN A 151 | 23.735 | 8.497  | 36.260 | 1.00 | 30.09 | O |
| ATOM | 1108 | ND2 | ASN A 151 | 23.991 | 10.611 | 36.930 | 1.00 | 29.31 | N |
| ATOM | 1109 | N   | ASP A 152 | 26.020 | 6.999  | 34.627 | 1.00 | 30.27 | N |
| ATOM | 1110 | CA  | ASP A 152 | 26.034 | 5.514  | 34.649 | 1.00 | 30.85 | C |
| ATOM | 1111 | C   | ASP A 152 | 24.830 | 4.797  | 35.212 | 1.00 | 30.51 | C |
| ATOM | 1112 | O   | ASP A 152 | 24.779 | 3.562  | 35.137 | 1.00 | 30.29 | O |
| ATOM | 1113 | CB  | ASP A 152 | 27.178 | 4.965  | 35.519 | 1.00 | 31.48 | C |
| ATOM | 1114 | CG  | ASP A 152 | 28.384 | 5.812  | 35.493 | 1.00 | 34.64 | C |
| ATOM | 1115 | OD1 | ASP A 152 | 28.588 | 6.523  | 34.482 | 1.00 | 41.71 | O |
| ATOM | 1116 | OD2 | ASP A 152 | 29.177 | 5.857  | 36.437 | 1.00 | 37.31 | O |
| ATOM | 1117 | N   | THR A 153 | 23.894 | 5.501  | 35.833 | 1.00 | 30.21 | N |
| ATOM | 1118 | CA  | THR A 153 | 22.767 | 4.785  | 36.432 | 1.00 | 30.13 | C |
| ATOM | 1119 | C   | THR A 153 | 21.612 | 4.626  | 35.463 | 1.00 | 29.54 | C |
| ATOM | 1120 | O   | THR A 153 | 20.639 | 3.970  | 35.778 | 1.00 | 29.38 | O |
| ATOM | 1121 | CB  | THR A 153 | 22.277 | 5.481  | 37.704 | 1.00 | 30.37 | C |
| ATOM | 1122 | OG1 | THR A 153 | 21.735 | 6.770  | 37.373 | 1.00 | 31.06 | O |
| ATOM | 1123 | CG2 | THR A 153 | 23.452 | 5.763  | 38.658 | 1.00 | 30.56 | C |
| ATOM | 1124 | N   | VAL A 154 | 21.703 | 5.213  | 34.280 | 1.00 | 29.07 | N |
| ATOM | 1125 | CA  | VAL A 154 | 20.596 | 5.082  | 33.346 | 1.00 | 28.90 | C |
| ATOM | 1126 | C   | VAL A 154 | 20.488 | 3.613  | 32.968 | 1.00 | 28.83 | C |
| ATOM | 1127 | O   | VAL A 154 | 21.486 | 2.898  | 33.002 | 1.00 | 28.78 | O |
| ATOM | 1128 | CB  | VAL A 154 | 20.762 | 5.952  | 32.088 | 1.00 | 28.61 | C |
| ATOM | 1129 | CG1 | VAL A 154 | 20.808 | 7.410  | 32.462 | 1.00 | 29.14 | C |
| ATOM | 1130 | CG2 | VAL A 154 | 21.999 | 5.547  | 31.305 | 1.00 | 28.52 | C |
| ATOM | 1131 | N   | GLY A 155 | 19.283 | 3.170  | 32.615 | 1.00 | 28.74 | N |
| ATOM | 1132 | CA  | GLY A 155 | 19.043 | 1.780  | 32.263 | 1.00 | 28.33 | C |
| ATOM | 1133 | C   | GLY A 155 | 19.484 | 1.387  | 30.860 | 1.00 | 28.70 | C |
| ATOM | 1134 | O   | GLY A 155 | 19.862 | 2.235  | 30.031 | 1.00 | 28.27 | O |
| ATOM | 1135 | N   | ARG A 156 | 19.384 | 0.088  | 30.591 | 1.00 | 28.47 | N |
| ATOM | 1136 | CA  | ARG A 156 | 19.857 | -0.519 | 29.349 | 1.00 | 28.54 | C |
| ATOM | 1137 | C   | ARG A 156 | 19.291 | 0.096  | 28.084 | 1.00 | 28.18 | C |
| ATOM | 1138 | O   | ARG A 156 | 20.029 | 0.346  | 27.143 | 1.00 | 28.69 | O |
| ATOM | 1139 | CB  | ARG A 156 | 19.582 | -2.019 | 29.362 | 1.00 | 28.58 | C |
| ATOM | 1140 | N   | LYS A 157 | 17.986 | 0.304  | 28.042 | 1.00 | 27.53 | N |
| ATOM | 1141 | CA  | LYS A 157 | 17.390 | 0.888  | 26.860 | 1.00 | 27.32 | C |
| ATOM | 1142 | C   | LYS A 157 | 17.947 | 2.306  | 26.625 | 1.00 | 27.10 | C |
| ATOM | 1143 | O   | LYS A 157 | 18.213 | 2.672  | 25.490 | 1.00 | 26.76 | O |
| ATOM | 1144 | CB  | LYS A 157 | 15.858 | 0.902  | 26.960 | 1.00 | 27.68 | C |
| ATOM | 1145 | CG  | LYS A 157 | 15.171 | -0.451 | 26.656 | 1.00 | 26.26 | C |
| ATOM | 1146 | N   | ILE A 158 | 18.138 | 3.086  | 27.688 | 1.00 | 26.68 | N |
| ATOM | 1147 | CA  | ILE A 158 | 18.665 | 4.450  | 27.543 | 1.00 | 26.67 | C |
| ATOM | 1148 | C   | ILE A 158 | 20.107 | 4.368  | 27.100 | 1.00 | 26.53 | C |
| ATOM | 1149 | O   | ILE A 158 | 20.558 | 5.170  | 26.285 | 1.00 | 25.74 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1150 | CB  | ILE | A | 158 | 18.570 | 5.245  | 28.837 | 1.00 | 26.51 | C |
| ATOM | 1151 | CG1 | ILE | A | 158 | 17.114 | 5.399  | 29.269 | 1.00 | 27.11 | C |
| ATOM | 1152 | CG2 | ILE | A | 158 | 19.208 | 6.618  | 28.667 | 1.00 | 27.55 | C |
| ATOM | 1153 | CD1 | ILE | A | 158 | 16.232 | 6.028  | 28.260 | 1.00 | 28.98 | C |
| ATOM | 1154 | N   | VAL | A | 159 | 20.817 | 3.378  | 27.629 | 1.00 | 26.46 | N |
| ATOM | 1155 | CA  | VAL | A | 159 | 22.187 | 3.125  | 27.226 | 1.00 | 26.70 | C |
| ATOM | 1156 | C   | VAL | A | 159 | 22.191 | 2.813  | 25.728 | 1.00 | 26.30 | C |
| ATOM | 1157 | O   | VAL | A | 159 | 23.022 | 3.332  | 24.999 | 1.00 | 25.90 | O |
| ATOM | 1158 | CB  | VAL | A | 159 | 22.819 | 1.963  | 28.018 | 1.00 | 27.18 | C |
| ATOM | 1159 | CG1 | VAL | A | 159 | 24.045 | 1.436  | 27.311 | 1.00 | 28.12 | C |
| ATOM | 1160 | CG2 | VAL | A | 159 | 23.180 | 2.410  | 29.427 | 1.00 | 27.44 | C |
| ATOM | 1161 | N   | MET | A | 160 | 21.255 | 1.984  | 25.269 | 1.00 | 26.08 | N |
| ATOM | 1162 | CA  | MET | A | 160 | 21.175 | 1.652  | 23.840 | 1.00 | 26.30 | C |
| ATOM | 1163 | C   | MET | A | 160 | 20.906 | 2.929  | 23.005 | 1.00 | 24.71 | C |
| ATOM | 1164 | O   | MET | A | 160 | 21.559 | 3.164  | 22.000 | 1.00 | 23.40 | O |
| ATOM | 1165 | CB  | MET | A | 160 | 20.081 | 0.617  | 23.565 | 1.00 | 26.71 | C |
| ATOM | 1166 | CG  | MET | A | 160 | 20.401 | -0.790 | 24.070 | 1.00 | 30.23 | C |
| ATOM | 1167 | SD  | MET | A | 160 | 21.721 | -1.628 | 23.154 | 1.00 | 35.73 | S |
| ATOM | 1168 | CE  | MET | A | 160 | 20.883 | -1.823 | 21.524 | 1.00 | 36.68 | C |
| ATOM | 1169 | N   | ASP | A | 161 | 19.948 | 3.739  | 23.439 | 1.00 | 23.86 | N |
| ATOM | 1170 | CA  | ASP | A | 161 | 19.636 | 5.000  | 22.756 | 1.00 | 23.67 | C |
| ATOM | 1171 | C   | ASP | A | 161 | 20.840 | 5.943  | 22.664 | 1.00 | 22.65 | C |
| ATOM | 1172 | O   | ASP | A | 161 | 21.148 | 6.478  | 21.593 | 1.00 | 23.02 | O |
| ATOM | 1173 | CB  | ASP | A | 161 | 18.472 | 5.699  | 23.455 | 1.00 | 23.42 | C |
| ATOM | 1174 | CG  | ASP | A | 161 | 17.178 | 4.898  | 23.369 | 1.00 | 24.19 | C |
| ATOM | 1175 | OD1 | ASP | A | 161 | 17.095 | 3.941  | 22.552 | 1.00 | 19.47 | O |
| ATOM | 1176 | OD2 | ASP | A | 161 | 16.197 | 5.164  | 24.087 | 1.00 | 24.90 | O |
| ATOM | 1177 | N   | PHE | A | 162 | 21.513 | 6.132  | 23.791 | 1.00 | 21.70 | N |
| ATOM | 1178 | CA  | PHE | A | 162 | 22.667 | 7.003  | 23.903 | 1.00 | 21.16 | C |
| ATOM | 1179 | C   | PHE | A | 162 | 23.777 | 6.557  | 22.964 | 1.00 | 20.02 | C |
| ATOM | 1180 | O   | PHE | A | 162 | 24.393 | 7.362  | 22.310 | 1.00 | 20.22 | O |
| ATOM | 1181 | CB  | PHE | A | 162 | 23.144 | 7.010  | 25.364 | 1.00 | 21.38 | C |
| ATOM | 1182 | CG  | PHE | A | 162 | 24.286 | 7.936  | 25.650 | 1.00 | 22.82 | C |
| ATOM | 1183 | CD1 | PHE | A | 162 | 24.072 | 9.290  | 25.882 | 1.00 | 26.05 | C |
| ATOM | 1184 | CD2 | PHE | A | 162 | 25.579 | 7.450  | 25.738 | 1.00 | 24.99 | C |
| ATOM | 1185 | CE1 | PHE | A | 162 | 25.144 | 10.136 | 26.181 | 1.00 | 25.32 | C |
| ATOM | 1186 | CE2 | PHE | A | 162 | 26.654 | 8.301  | 26.026 | 1.00 | 24.73 | C |
| ATOM | 1187 | CZ  | PHE | A | 162 | 26.438 | 9.622  | 26.250 | 1.00 | 24.82 | C |
| ATOM | 1188 | N   | LEU | A | 163 | 24.029 | 5.271  | 22.894 | 1.00 | 19.74 | N |
| ATOM | 1189 | CA  | LEU | A | 163 | 25.064 | 4.767  | 21.998 | 1.00 | 19.88 | C |
| ATOM | 1190 | C   | LEU | A | 163 | 24.688 | 4.965  | 20.533 | 1.00 | 18.90 | C |
| ATOM | 1191 | O   | LEU | A | 163 | 25.554 | 5.020  | 19.675 | 1.00 | 18.20 | O |
| ATOM | 1192 | CB  | LEU | A | 163 | 25.320 | 3.287  | 22.256 | 1.00 | 19.78 | C |
| ATOM | 1193 | CG  | LEU | A | 163 | 26.078 | 3.019  | 23.546 | 1.00 | 20.79 | C |
| ATOM | 1194 | CD1 | LEU | A | 163 | 26.069 | 1.534  | 23.811 | 1.00 | 21.16 | C |
| ATOM | 1195 | CD2 | LEU | A | 163 | 27.498 | 3.567  | 23.456 | 1.00 | 21.66 | C |
| ATOM | 1196 | N   | GLY | A | 164 | 23.395 | 5.055  | 20.272 | 1.00 | 18.33 | N |
| ATOM | 1197 | CA  | GLY | A | 164 | 22.883 | 5.296  | 18.941 | 1.00 | 19.05 | C |
| ATOM | 1198 | C   | GLY | A | 164 | 22.879 | 6.764  | 18.519 | 1.00 | 19.33 | C |
| ATOM | 1199 | O   | GLY | A | 164 | 22.347 | 7.079  | 17.451 | 1.00 | 20.16 | O |
| ATOM | 1200 | N   | PHE | A | 165 | 23.424 | 7.651  | 19.350 | 1.00 | 18.45 | N |
| ATOM | 1201 | CA  | PHE | A | 165 | 23.516 | 9.048  | 18.974 | 1.00 | 19.26 | C |
| ATOM | 1202 | C   | PHE | A | 165 | 24.548 | 9.102  | 17.850 | 1.00 | 19.34 | C |
| ATOM | 1203 | O   | PHE | A | 165 | 25.363 | 8.177  | 17.720 | 1.00 | 18.77 | O |
| ATOM | 1204 | CB  | PHE | A | 165 | 23.947 | 9.915  | 20.158 | 1.00 | 19.09 | C |
| ATOM | 1205 | CG  | PHE | A | 165 | 22.862 | 10.139 | 21.208 | 1.00 | 20.44 | C |
| ATOM | 1206 | CD1 | PHE | A | 165 | 21.572 | 9.632  | 21.047 | 1.00 | 21.56 | C |
| ATOM | 1207 | CD2 | PHE | A | 165 | 23.143 | 10.878 | 22.357 | 1.00 | 20.27 | C |
| ATOM | 1208 | CE1 | PHE | A | 165 | 20.604 | 9.840  | 22.010 | 1.00 | 21.01 | C |
| ATOM | 1209 | CE2 | PHE | A | 165 | 22.174 | 11.096 | 23.326 | 1.00 | 20.14 | C |
| ATOM | 1210 | CZ  | PHE | A | 165 | 20.913 | 10.567 | 23.163 | 1.00 | 22.00 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1211 | N   | ASN | A | 166 | 24.508 | 10.157 | 17.040 | 1.00 | 19.48 | N |
| ATOM | 1212 | CA  | ASN | A | 166 | 25.428 | 10.290 | 15.897 | 1.00 | 20.08 | C |
| ATOM | 1213 | C   | ASN | A | 166 | 26.827 | 10.792 | 16.305 | 1.00 | 20.53 | C |
| ATOM | 1214 | O   | ASN | A | 166 | 27.193 | 11.975 | 16.076 | 1.00 | 20.34 | O |
| ATOM | 1215 | CB  | ASN | A | 166 | 24.836 | 11.183 | 14.790 | 1.00 | 19.52 | C |
| ATOM | 1216 | CG  | ASN | A | 166 | 25.572 | 11.003 | 13.451 | 1.00 | 19.82 | C |
| ATOM | 1217 | OD1 | ASN | A | 166 | 26.652 | 10.376 | 13.412 | 1.00 | 18.39 | O |
| ATOM | 1218 | ND2 | ASN | A | 166 | 24.987 | 11.528 | 12.350 | 1.00 | 15.25 | N |
| ATOM | 1219 | N   | TRP | A | 167 | 27.564 | 9.892  | 16.955 | 1.00 | 20.69 | N |
| ATOM | 1220 | CA  | TRP | A | 167 | 28.911 | 10.161 | 17.441 | 1.00 | 21.20 | C |
| ATOM | 1221 | C   | TRP | A | 167 | 29.858 | 10.404 | 16.270 | 1.00 | 21.35 | C |
| ATOM | 1222 | O   | TRP | A | 167 | 30.806 | 11.171 | 16.371 | 1.00 | 21.36 | O |
| ATOM | 1223 | CB  | TRP | A | 167 | 29.402 | 8.977  | 18.316 | 1.00 | 21.31 | C |
| ATOM | 1224 | CG  | TRP | A | 167 | 28.550 | 8.849  | 19.539 | 1.00 | 21.63 | C |
| ATOM | 1225 | CD1 | TRP | A | 167 | 27.673 | 7.841  | 19.844 | 1.00 | 22.35 | C |
| ATOM | 1226 | CD2 | TRP | A | 167 | 28.433 | 9.808  | 20.591 | 1.00 | 20.88 | C |
| ATOM | 1227 | NE1 | TRP | A | 167 | 27.030 | 8.119  | 21.028 | 1.00 | 22.98 | N |
| ATOM | 1228 | CE2 | TRP | A | 167 | 27.486 | 9.315  | 21.511 | 1.00 | 21.22 | C |
| ATOM | 1229 | CE3 | TRP | A | 167 | 29.054 | 11.036 | 20.863 | 1.00 | 20.14 | C |
| ATOM | 1230 | CZ2 | TRP | A | 167 | 27.143 | 9.999  | 22.670 | 1.00 | 22.17 | C |
| ATOM | 1231 | CZ3 | TRP | A | 167 | 28.693 | 11.724 | 21.990 | 1.00 | 19.81 | C |
| ATOM | 1232 | CH2 | TRP | A | 167 | 27.742 | 11.206 | 22.889 | 1.00 | 21.02 | C |
| ATOM | 1233 | N   | ASN | A | 168 | 29.610 | 9.743  | 15.153 | 1.00 | 21.50 | N |
| ATOM | 1234 | CA  | ASN | A | 168 | 30.464 | 9.927  | 13.991 | 1.00 | 21.77 | C |
| ATOM | 1235 | C   | ASN | A | 168 | 30.488 | 11.406 | 13.605 | 1.00 | 21.48 | C |
| ATOM | 1236 | O   | ASN | A | 168 | 31.549 | 11.992 | 13.428 | 1.00 | 20.55 | O |
| ATOM | 1237 | CB  | ASN | A | 168 | 29.964 | 9.101  | 12.814 | 1.00 | 22.00 | C |
| ATOM | 1238 | CG  | ASN | A | 168 | 30.856 | 9.236  | 11.584 | 1.00 | 23.99 | C |
| ATOM | 1239 | OD1 | ASN | A | 168 | 32.052 | 8.974  | 11.661 | 1.00 | 26.79 | O |
| ATOM | 1240 | ND2 | ASN | A | 168 | 30.277 | 9.652  | 10.448 | 1.00 | 24.40 | N |
| ATOM | 1241 | N   | TRP | A | 169 | 29.302 | 11.995 | 13.484 | 1.00 | 21.28 | N |
| ATOM | 1242 | CA  | TRP | A | 169 | 29.183 | 13.372 | 13.071 | 1.00 | 21.23 | C |
| ATOM | 1243 | C   | TRP | A | 169 | 29.708 | 14.331 | 14.133 | 1.00 | 21.44 | C |
| ATOM | 1244 | O   | TRP | A | 169 | 30.450 | 15.258 | 13.822 | 1.00 | 20.50 | O |
| ATOM | 1245 | CB  | TRP | A | 169 | 27.736 | 13.741 | 12.740 | 1.00 | 21.29 | C |
| ATOM | 1246 | CG  | TRP | A | 169 | 27.611 | 15.186 | 12.397 | 1.00 | 20.56 | C |
| ATOM | 1247 | CD1 | TRP | A | 169 | 27.840 | 15.766 | 11.173 | 1.00 | 19.81 | C |
| ATOM | 1248 | CD2 | TRP | A | 169 | 27.293 | 16.256 | 13.290 | 1.00 | 20.58 | C |
| ATOM | 1249 | NE1 | TRP | A | 169 | 27.641 | 17.124 | 11.253 | 1.00 | 20.45 | N |
| ATOM | 1250 | CE2 | TRP | A | 169 | 27.313 | 17.453 | 12.540 | 1.00 | 21.52 | C |
| ATOM | 1251 | CE3 | TRP | A | 169 | 26.951 | 16.324 | 14.636 | 1.00 | 22.34 | C |
| ATOM | 1252 | CZ2 | TRP | A | 169 | 27.036 | 18.705 | 13.102 | 1.00 | 24.24 | C |
| ATOM | 1253 | CZ3 | TRP | A | 169 | 26.690 | 17.558 | 15.195 | 1.00 | 24.93 | C |
| ATOM | 1254 | CH2 | TRP | A | 169 | 26.728 | 18.736 | 14.423 | 1.00 | 25.53 | C |
| ATOM | 1255 | N   | ILE | A | 170 | 29.318 | 14.124 | 15.381 | 1.00 | 21.81 | N |
| ATOM | 1256 | CA  | ILE | A | 170 | 29.742 | 15.056 | 16.412 | 1.00 | 22.51 | C |
| ATOM | 1257 | C   | ILE | A | 170 | 31.245 | 14.894 | 16.755 | 1.00 | 23.07 | C |
| ATOM | 1258 | O   | ILE | A | 170 | 31.917 | 15.872 | 17.067 | 1.00 | 23.88 | O |
| ATOM | 1259 | CB  | ILE | A | 170 | 28.837 | 14.988 | 17.662 | 1.00 | 21.97 | C |
| ATOM | 1260 | CG1 | ILE | A | 170 | 28.878 | 16.326 | 18.396 | 1.00 | 21.44 | C |
| ATOM | 1261 | CG2 | ILE | A | 170 | 29.262 | 13.894 | 18.581 | 1.00 | 21.76 | C |
| ATOM | 1262 | CD1 | ILE | A | 170 | 27.794 | 16.472 | 19.409 | 1.00 | 21.59 | C |
| ATOM | 1263 | N   | ASN | A | 171 | 31.781 | 13.692 | 16.674 | 1.00 | 23.52 | N |
| ATOM | 1264 | CA  | ASN | A | 171 | 33.209 | 13.516 | 16.934 | 1.00 | 24.55 | C |
| ATOM | 1265 | C   | ASN | A | 171 | 34.021 | 14.254 | 15.874 | 1.00 | 25.23 | C |
| ATOM | 1266 | O   | ASN | A | 171 | 35.067 | 14.828 | 16.171 | 1.00 | 25.14 | O |
| ATOM | 1267 | CB  | ASN | A | 171 | 33.626 | 12.031 | 16.949 | 1.00 | 24.52 | C |
| ATOM | 1268 | CG  | ASN | A | 171 | 33.095 | 11.271 | 18.171 | 1.00 | 24.45 | C |
| ATOM | 1269 | OD1 | ASN | A | 171 | 32.625 | 11.855 | 19.154 | 1.00 | 23.01 | O |
| ATOM | 1270 | ND2 | ASN | A | 171 | 33.169 | 9.969  | 18.099 | 1.00 | 22.49 | N |
| ATOM | 1271 | N   | LYS | A | 172 | 33.560 | 14.219 | 14.630 | 1.00 | 25.46 | N |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1272 | CA  | LYS | A | 172 | 34.255 | 14.963 | 13.592 | 1.00 | 26.46 | C |
| ATOM | 1273 | C   | LYS | A | 172 | 34.221 | 16.478 | 13.873 | 1.00 | 25.77 | C |
| ATOM | 1274 | O   | LYS | A | 172 | 35.224 | 17.169 | 13.681 | 1.00 | 25.85 | O |
| ATOM | 1275 | CB  | LYS | A | 172 | 33.705 | 14.634 | 12.205 | 1.00 | 26.90 | C |
| ATOM | 1276 | CG  | LYS | A | 172 | 34.262 | 13.351 | 11.668 | 1.00 | 29.88 | C |
| ATOM | 1277 | CD  | LYS | A | 172 | 33.752 | 13.033 | 10.240 | 1.00 | 34.20 | C |
| ATOM | 1278 | CE  | LYS | A | 172 | 34.458 | 11.810 | 9.690  | 1.00 | 36.15 | C |
| ATOM | 1279 | NZ  | LYS | A | 172 | 34.556 | 11.800 | 8.188  | 1.00 | 40.56 | N |
| ATOM | 1280 | N   | GLN | A | 173 | 33.088 | 16.986 | 14.338 | 1.00 | 25.37 | N |
| ATOM | 1281 | CA  | GLN | A | 173 | 32.981 | 18.400 | 14.690 | 1.00 | 25.52 | C |
| ATOM | 1282 | C   | GLN | A | 173 | 34.002 | 18.741 | 15.774 | 1.00 | 25.71 | C |
| ATOM | 1283 | O   | GLN | A | 173 | 34.780 | 19.669 | 15.618 | 1.00 | 26.05 | O |
| ATOM | 1284 | CB  | GLN | A | 173 | 31.589 | 18.740 | 15.200 | 1.00 | 25.30 | C |
| ATOM | 1285 | CG  | GLN | A | 173 | 30.522 | 18.729 | 14.138 | 1.00 | 25.28 | C |
| ATOM | 1286 | CD  | GLN | A | 173 | 30.783 | 19.753 | 13.061 | 1.00 | 26.34 | C |
| ATOM | 1287 | OE1 | GLN | A | 173 | 31.252 | 20.872 | 13.345 | 1.00 | 26.57 | O |
| ATOM | 1288 | NE2 | GLN | A | 173 | 30.492 | 19.386 | 11.822 | 1.00 | 23.68 | N |
| ATOM | 1289 | N   | GLN | A | 174 | 33.972 | 17.985 | 16.867 | 1.00 | 25.20 | N |
| ATOM | 1290 | CA  | GLN | A | 174 | 34.931 | 18.124 | 17.944 | 1.00 | 25.45 | C |
| ATOM | 1291 | C   | GLN | A | 174 | 36.380 | 18.182 | 17.392 | 1.00 | 25.74 | C |
| ATOM | 1292 | O   | GLN | A | 174 | 37.152 | 19.066 | 17.767 | 1.00 | 24.76 | O |
| ATOM | 1293 | CB  | GLN | A | 174 | 34.770 | 16.951 | 18.923 | 1.00 | 25.13 | C |
| ATOM | 1294 | CG  | GLN | A | 174 | 35.771 | 16.925 | 20.048 | 1.00 | 26.00 | C |
| ATOM | 1295 | CD  | GLN | A | 174 | 35.636 | 15.697 | 20.929 | 1.00 | 26.76 | C |
| ATOM | 1296 | OE1 | GLN | A | 174 | 35.278 | 14.629 | 20.450 | 1.00 | 28.02 | O |
| ATOM | 1297 | NE2 | GLN | A | 174 | 35.917 | 15.851 | 22.222 | 1.00 | 26.75 | N |
| ATOM | 1298 | N   | GLY | A | 175 | 36.724 | 17.249 | 16.505 | 1.00 | 25.61 | N |
| ATOM | 1299 | CA  | GLY | A | 175 | 38.040 | 17.201 | 15.887 | 1.00 | 26.56 | C |
| ATOM | 1300 | C   | GLY | A | 175 | 38.333 | 18.393 | 14.980 | 1.00 | 27.62 | C |
| ATOM | 1301 | O   | GLY | A | 175 | 39.371 | 19.051 | 15.111 | 1.00 | 28.21 | O |
| ATOM | 1302 | N   | LYS | A | 176 | 37.415 | 18.695 | 14.074 | 1.00 | 28.41 | N |
| ATOM | 1303 | CA  | LYS | A | 176 | 37.583 | 19.834 | 13.173 | 1.00 | 29.52 | C |
| ATOM | 1304 | C   | LYS | A | 176 | 37.778 | 21.177 | 13.895 | 1.00 | 29.38 | C |
| ATOM | 1305 | O   | LYS | A | 176 | 38.557 | 22.009 | 13.443 | 1.00 | 29.30 | O |
| ATOM | 1306 | CB  | LYS | A | 176 | 36.371 | 19.977 | 12.257 | 1.00 | 29.90 | C |
| ATOM | 1307 | CG  | LYS | A | 176 | 36.212 | 18.895 | 11.227 | 1.00 | 32.69 | C |
| ATOM | 1308 | CD  | LYS | A | 176 | 35.023 | 19.242 | 10.336 | 1.00 | 36.10 | C |
| ATOM | 1309 | CE  | LYS | A | 176 | 34.114 | 18.065 | 10.148 | 1.00 | 37.89 | C |
| ATOM | 1310 | NZ  | LYS | A | 176 | 32.736 | 18.469 | 9.746  | 1.00 | 40.12 | N |
| ATOM | 1311 | N   | ARG | A | 177 | 37.060 | 21.397 | 14.993 | 1.00 | 29.00 | N |
| ATOM | 1312 | CA  | ARG | A | 177 | 37.164 | 22.671 | 15.710 | 1.00 | 29.17 | C |
| ATOM | 1313 | C   | ARG | A | 177 | 38.260 | 22.741 | 16.781 | 1.00 | 28.13 | C |
| ATOM | 1314 | O   | ARG | A | 177 | 38.433 | 23.788 | 17.394 | 1.00 | 27.46 | O |
| ATOM | 1315 | CB  | ARG | A | 177 | 35.831 | 23.025 | 16.391 | 1.00 | 29.67 | C |
| ATOM | 1316 | CG  | ARG | A | 177 | 34.606 | 22.876 | 15.536 | 1.00 | 31.86 | C |
| ATOM | 1317 | CD  | ARG | A | 177 | 34.629 | 23.648 | 14.243 | 1.00 | 35.68 | C |
| ATOM | 1318 | NE  | ARG | A | 177 | 33.691 | 23.034 | 13.313 | 1.00 | 38.08 | N |
| ATOM | 1319 | CZ  | ARG | A | 177 | 33.865 | 22.938 | 12.015 | 1.00 | 40.57 | C |
| ATOM | 1320 | NH1 | ARG | A | 177 | 34.958 | 23.420 | 11.436 | 1.00 | 41.44 | N |
| ATOM | 1321 | NH2 | ARG | A | 177 | 32.927 | 22.362 | 11.283 | 1.00 | 42.98 | N |
| ATOM | 1322 | N   | GLY | A | 178 | 38.972 | 21.640 | 17.014 | 1.00 | 27.36 | N |
| ATOM | 1323 | CA  | GLY | A | 178 | 40.013 | 21.589 | 18.028 | 1.00 | 26.75 | C |
| ATOM | 1324 | C   | GLY | A | 178 | 39.460 | 21.655 | 19.444 | 1.00 | 26.55 | C |
| ATOM | 1325 | O   | GLY | A | 178 | 40.175 | 21.999 | 20.394 | 1.00 | 27.31 | O |
| ATOM | 1326 | N   | TRP | A | 179 | 38.195 | 21.308 | 19.620 | 1.00 | 25.19 | N |
| ATOM | 1327 | CA  | TRP | A | 179 | 37.626 | 21.379 | 20.947 | 1.00 | 25.17 | C |
| ATOM | 1328 | C   | TRP | A | 179 | 38.257 | 20.404 | 21.926 | 1.00 | 25.28 | C |
| ATOM | 1329 | O   | TRP | A | 179 | 38.909 | 19.454 | 21.541 | 1.00 | 24.67 | O |
| ATOM | 1330 | CB  | TRP | A | 179 | 36.127 | 21.139 | 20.901 | 1.00 | 24.78 | C |
| ATOM | 1331 | CG  | TRP | A | 179 | 35.364 | 22.197 | 20.201 | 1.00 | 24.55 | C |
| ATOM | 1332 | CD1 | TRP | A | 179 | 35.830 | 23.425 | 19.776 | 1.00 | 23.00 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1333 | CD2 | TRP | A | 179 | 33.985 | 22.140 | 19.825 | 1.00 | 24.35 | C |
| ATOM | 1334 | NE1 | TRP | A | 179 | 34.822 | 24.122 | 19.153 | 1.00 | 24.53 | N |
| ATOM | 1335 | CE2 | TRP | A | 179 | 33.676 | 23.355 | 19.167 | 1.00 | 24.34 | C |
| ATOM | 1336 | CE3 | TRP | A | 179 | 32.982 | 21.177 | 19.957 | 1.00 | 23.62 | C |
| ATOM | 1337 | CZ2 | TRP | A | 179 | 32.417 | 23.627 | 18.659 | 1.00 | 22.63 | C |
| ATOM | 1338 | CZ3 | TRP | A | 179 | 31.726 | 21.454 | 19.442 | 1.00 | 24.07 | C |
| ATOM | 1339 | CH2 | TRP | A | 179 | 31.453 | 22.674 | 18.811 | 1.00 | 23.17 | C |
| ATOM | 1340 | N   | GLY | A | 180 | 38.061 | 20.669 | 23.210 | 1.00 | 25.61 | N |
| ATOM | 1341 | CA  | GLY | A | 180 | 38.471 | 19.737 | 24.240 | 1.00 | 25.44 | C |
| ATOM | 1342 | C   | GLY | A | 180 | 37.428 | 18.634 | 24.377 | 1.00 | 26.09 | C |
| ATOM | 1343 | O   | GLY | A | 180 | 36.592 | 18.432 | 23.491 | 1.00 | 26.60 | O |
| ATOM | 1344 | N   | GLN | A | 181 | 37.448 | 17.934 | 25.503 | 1.00 | 26.33 | N |
| ATOM | 1345 | CA  | GLN | A | 181 | 36.561 | 16.806 | 25.708 | 1.00 | 26.77 | C |
| ATOM | 1346 | C   | GLN | A | 181 | 35.099 | 17.180 | 25.953 | 1.00 | 26.26 | C |
| ATOM | 1347 | O   | GLN | A | 181 | 34.775 | 18.291 | 26.371 | 1.00 | 25.90 | O |
| ATOM | 1348 | CB  | GLN | A | 181 | 37.044 | 15.970 | 26.887 | 1.00 | 27.12 | C |
| ATOM | 1349 | CG  | GLN | A | 181 | 36.689 | 16.543 | 28.269 | 1.00 | 29.66 | C |
| ATOM | 1350 | CD  | GLN | A | 181 | 36.917 | 15.533 | 29.388 | 1.00 | 33.17 | C |
| ATOM | 1351 | OE1 | GLN | A | 181 | 38.055 | 15.295 | 29.791 | 1.00 | 35.52 | O |
| ATOM | 1352 | NE2 | GLN | A | 181 | 35.839 | 14.920 | 29.869 | 1.00 | 35.59 | N |
| ATOM | 1353 | N   | LEU | A | 182 | 34.238 | 16.225 | 25.646 | 1.00 | 25.83 | N |
| ATOM | 1354 | CA  | LEU | A | 182 | 32.831 | 16.241 | 26.021 | 1.00 | 25.59 | C |
| ATOM | 1355 | C   | LEU | A | 182 | 32.850 | 16.162 | 27.543 | 1.00 | 24.45 | C |
| ATOM | 1356 | O   | LEU | A | 182 | 33.433 | 15.209 | 28.084 | 1.00 | 23.27 | O |
| ATOM | 1357 | CB  | LEU | A | 182 | 32.180 | 14.958 | 25.499 | 1.00 | 25.74 | C |
| ATOM | 1358 | CG  | LEU | A | 182 | 30.666 | 14.790 | 25.403 | 1.00 | 28.29 | C |
| ATOM | 1359 | CD1 | LEU | A | 182 | 30.276 | 13.328 | 25.676 | 1.00 | 27.13 | C |
| ATOM | 1360 | CD2 | LEU | A | 182 | 29.928 | 15.671 | 26.303 | 1.00 | 30.64 | C |
| ATOM | 1361 | N   | THR | A | 183 | 32.288 | 17.158 | 28.239 | 1.00 | 23.24 | N |
| ATOM | 1362 | CA  | THR | A | 183 | 32.256 | 17.110 | 29.699 | 1.00 | 22.37 | C |
| ATOM | 1363 | C   | THR | A | 183 | 30.956 | 16.504 | 30.150 | 1.00 | 22.01 | C |
| ATOM | 1364 | O   | THR | A | 183 | 30.907 | 15.867 | 31.186 | 1.00 | 21.99 | O |
| ATOM | 1365 | CB  | THR | A | 183 | 32.395 | 18.504 | 30.371 | 1.00 | 22.62 | C |
| ATOM | 1366 | OG1 | THR | A | 183 | 31.367 | 19.393 | 29.893 | 1.00 | 20.93 | O |
| ATOM | 1367 | CG2 | THR | A | 183 | 33.707 | 19.154 | 30.013 | 1.00 | 22.33 | C |
| ATOM | 1368 | N   | SER | A | 184 | 29.885 | 16.711 | 29.396 | 1.00 | 21.54 | N |
| ATOM | 1369 | CA  | SER | A | 184 | 28.622 | 16.146 | 29.810 | 1.00 | 21.58 | C |
| ATOM | 1370 | C   | SER | A | 184 | 27.498 | 16.381 | 28.866 | 1.00 | 21.50 | C |
| ATOM | 1371 | O   | SER | A | 184 | 27.610 | 17.168 | 27.928 | 1.00 | 21.85 | O |
| ATOM | 1372 | CB  | SER | A | 184 | 28.209 | 16.715 | 31.158 | 1.00 | 21.78 | C |
| ATOM | 1373 | OG  | SER | A | 184 | 27.856 | 18.072 | 31.056 | 1.00 | 23.20 | O |
| ATOM | 1374 | N   | ASN | A | 185 | 26.416 | 15.667 | 29.134 | 1.00 | 21.14 | N |
| ATOM | 1375 | CA  | ASN | A | 185 | 25.167 | 15.807 | 28.427 | 1.00 | 22.40 | C |
| ATOM | 1376 | C   | ASN | A | 185 | 24.104 | 16.059 | 29.459 | 1.00 | 22.16 | C |
| ATOM | 1377 | O   | ASN | A | 185 | 23.802 | 15.189 | 30.272 | 1.00 | 22.11 | O |
| ATOM | 1378 | CB  | ASN | A | 185 | 24.794 | 14.523 | 27.664 | 1.00 | 22.46 | C |
| ATOM | 1379 | CG  | ASN | A | 185 | 25.798 | 14.174 | 26.604 | 1.00 | 23.64 | C |
| ATOM | 1380 | OD1 | ASN | A | 185 | 26.582 | 13.257 | 26.789 | 1.00 | 25.26 | O |
| ATOM | 1381 | ND2 | ASN | A | 185 | 25.794 | 14.907 | 25.494 | 1.00 | 22.02 | N |
| ATOM | 1382 | N   | LEU | A | 186 | 23.507 | 17.228 | 29.391 | 1.00 | 22.02 | N |
| ATOM | 1383 | CA  | LEU | A | 186 | 22.461 | 17.600 | 30.319 | 1.00 | 22.34 | C |
| ATOM | 1384 | C   | LEU | A | 186 | 21.114 | 17.251 | 29.707 | 1.00 | 22.21 | C |
| ATOM | 1385 | O   | LEU | A | 186 | 20.808 | 17.623 | 28.582 | 1.00 | 22.59 | O |
| ATOM | 1386 | CB  | LEU | A | 186 | 22.519 | 19.111 | 30.591 | 1.00 | 22.36 | C |
| ATOM | 1387 | CG  | LEU | A | 186 | 21.650 | 19.642 | 31.739 | 1.00 | 23.03 | C |
| ATOM | 1388 | CD1 | LEU | A | 186 | 22.124 | 19.073 | 33.069 | 1.00 | 22.66 | C |
| ATOM | 1389 | CD2 | LEU | A | 186 | 21.636 | 21.213 | 31.782 | 1.00 | 21.88 | C |
| ATOM | 1390 | N   | LEU | A | 187 | 20.307 | 16.530 | 30.461 | 1.00 | 22.39 | N |
| ATOM | 1391 | CA  | LEU | A | 187 | 18.949 | 16.234 | 30.057 | 1.00 | 21.93 | C |
| ATOM | 1392 | C   | LEU | A | 187 | 18.089 | 17.336 | 30.659 | 1.00 | 21.94 | C |
| ATOM | 1393 | O   | LEU | A | 187 | 18.163 | 17.569 | 31.870 | 1.00 | 21.56 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1394 | CB  | LEU | A | 187 | 18.525 | 14.883 | 30.604 | 1.00 | 21.36 | C |
| ATOM | 1395 | CG  | LEU | A | 187 | 17.037 | 14.555 | 30.489 | 1.00 | 22.46 | C |
| ATOM | 1396 | CD1 | LEU | A | 187 | 16.550 | 14.530 | 29.038 | 1.00 | 22.25 | C |
| ATOM | 1397 | CD2 | LEU | A | 187 | 16.783 | 13.200 | 31.154 | 1.00 | 22.25 | C |
| ATOM | 1398 | N   | LEU | A | 188 | 17.301 | 18.028 | 29.826 | 1.00 | 21.68 | N |
| ATOM | 1399 | CA  | LEU | A | 188 | 16.400 | 19.052 | 30.329 | 1.00 | 22.46 | C |
| ATOM | 1400 | C   | LEU | A | 188 | 14.925 | 18.743 | 30.021 | 1.00 | 22.70 | C |
| ATOM | 1401 | O   | LEU | A | 188 | 14.511 | 18.622 | 28.864 | 1.00 | 23.01 | O |
| ATOM | 1402 | CB  | LEU | A | 188 | 16.747 | 20.432 | 29.769 | 1.00 | 22.51 | C |
| ATOM | 1403 | CG  | LEU | A | 188 | 18.166 | 20.932 | 29.998 | 1.00 | 24.09 | C |
| ATOM | 1404 | CD1 | LEU | A | 188 | 18.916 | 20.996 | 28.697 | 1.00 | 26.99 | C |
| ATOM | 1405 | CD2 | LEU | A | 188 | 18.135 | 22.308 | 30.564 | 1.00 | 25.94 | C |
| ATOM | 1406 | N   | ILE | A | 189 | 14.117 | 18.652 | 31.061 | 1.00 | 22.31 | N |
| ATOM | 1407 | CA  | ILE | A | 189 | 12.721 | 18.383 | 30.851 | 1.00 | 22.23 | C |
| ATOM | 1408 | C   | ILE | A | 189 | 11.959 | 19.459 | 31.554 | 1.00 | 22.43 | C |
| ATOM | 1409 | O   | ILE | A | 189 | 12.045 | 19.599 | 32.773 | 1.00 | 22.44 | O |
| ATOM | 1410 | CB  | ILE | A | 189 | 12.328 | 17.009 | 31.369 | 1.00 | 21.56 | C |
| ATOM | 1411 | CG1 | ILE | A | 189 | 13.178 | 15.944 | 30.695 | 1.00 | 21.26 | C |
| ATOM | 1412 | CG2 | ILE | A | 189 | 10.873 | 16.794 | 31.078 | 1.00 | 21.74 | C |
| ATOM | 1413 | CD1 | ILE | A | 189 | 12.851 | 14.481 | 31.136 | 1.00 | 22.52 | C |
| ATOM | 1414 | N   | GLY | A | 190 | 11.226 | 20.239 | 30.770 | 1.00 | 23.11 | N |
| ATOM | 1415 | CA  | GLY | A | 190 | 10.545 | 21.396 | 31.294 | 1.00 | 23.06 | C |
| ATOM | 1416 | C   | GLY | A | 190 | 9.084  | 21.395 | 30.988 | 1.00 | 23.56 | C |
| ATOM | 1417 | O   | GLY | A | 190 | 8.594  | 20.646 | 30.117 | 1.00 | 23.29 | O |
| ATOM | 1418 | N   | MET | A | 191 | 8.385  | 22.224 | 31.755 | 1.00 | 24.04 | N |
| ATOM | 1419 | CA  | MET | A | 191 | 6.980  | 22.468 | 31.542 | 1.00 | 24.73 | C |
| ATOM | 1420 | C   | MET | A | 191 | 6.837  | 23.623 | 30.576 | 1.00 | 24.58 | C |
| ATOM | 1421 | O   | MET | A | 191 | 7.747  | 24.464 | 30.443 | 1.00 | 24.72 | O |
| ATOM | 1422 | CB  | MET | A | 191 | 6.301  | 22.821 | 32.860 | 1.00 | 25.52 | C |
| ATOM | 1423 | CG  | MET | A | 191 | 6.212  | 21.649 | 33.806 | 1.00 | 26.99 | C |
| ATOM | 1424 | SD  | MET | A | 191 | 5.710  | 22.122 | 35.447 | 1.00 | 30.62 | S |
| ATOM | 1425 | CE  | MET | A | 191 | 4.076  | 22.639 | 35.135 | 1.00 | 32.05 | C |
| ATOM | 1426 | N   | GLU | A | 192 | 5.701  | 23.659 | 29.893 | 1.00 | 24.37 | N |
| ATOM | 1427 | CA  | GLU | A | 192 | 5.407  | 24.718 | 28.940 | 1.00 | 24.51 | C |
| ATOM | 1428 | C   | GLU | A | 192 | 5.468  | 26.072 | 29.628 | 1.00 | 24.20 | C |
| ATOM | 1429 | O   | GLU | A | 192 | 5.013  | 26.237 | 30.745 | 1.00 | 24.12 | O |
| ATOM | 1430 | CB  | GLU | A | 192 | 4.029  | 24.514 | 28.342 | 1.00 | 24.59 | C |
| ATOM | 1431 | CG  | GLU | A | 192 | 2.930  | 24.487 | 29.384 | 1.00 | 26.08 | C |
| ATOM | 1432 | CD  | GLU | A | 192 | 1.590  | 24.051 | 28.830 | 1.00 | 26.38 | C |
| ATOM | 1433 | OE1 | GLU | A | 192 | 1.530  | 23.568 | 27.676 | 1.00 | 27.04 | O |
| ATOM | 1434 | OE2 | GLU | A | 192 | 0.599  | 24.219 | 29.562 | 1.00 | 25.46 | O |
| ATOM | 1435 | N   | GLY | A | 193 | 6.045  | 27.051 | 28.962 | 1.00 | 24.44 | N |
| ATOM | 1436 | CA  | GLY | A | 193 | 6.153  | 28.364 | 29.562 | 1.00 | 24.21 | C |
| ATOM | 1437 | C   | GLY | A | 193 | 7.428  | 28.565 | 30.358 | 1.00 | 23.71 | C |
| ATOM | 1438 | O   | GLY | A | 193 | 7.728  | 29.691 | 30.697 | 1.00 | 24.97 | O |
| ATOM | 1439 | N   | ASN | A | 194 | 8.181  | 27.507 | 30.663 | 1.00 | 23.27 | N |
| ATOM | 1440 | CA  | ASN | A | 194 | 9.445  | 27.656 | 31.413 | 1.00 | 22.47 | C |
| ATOM | 1441 | C   | ASN | A | 194 | 10.465 | 28.476 | 30.636 | 1.00 | 22.35 | C |
| ATOM | 1442 | O   | ASN | A | 194 | 10.594 | 28.317 | 29.416 | 1.00 | 22.38 | O |
| ATOM | 1443 | CB  | ASN | A | 194 | 10.108 | 26.299 | 31.708 | 1.00 | 22.17 | C |
| ATOM | 1444 | CG  | ASN | A | 194 | 9.476  | 25.555 | 32.882 | 1.00 | 22.24 | C |
| ATOM | 1445 | OD1 | ASN | A | 194 | 8.477  | 25.992 | 33.453 | 1.00 | 23.81 | O |
| ATOM | 1446 | ND2 | ASN | A | 194 | 10.075 | 24.429 | 33.253 | 1.00 | 18.58 | N |
| ATOM | 1447 | N   | VAL | A | 195 | 11.226 | 29.295 | 31.362 | 1.00 | 21.64 | N |
| ATOM | 1448 | CA  | VAL | A | 195 | 12.263 | 30.114 | 30.789 | 1.00 | 21.41 | C |
| ATOM | 1449 | C   | VAL | A | 195 | 13.569 | 29.988 | 31.556 | 1.00 | 20.40 | C |
| ATOM | 1450 | O   | VAL | A | 195 | 13.603 | 30.014 | 32.790 | 1.00 | 20.03 | O |
| ATOM | 1451 | CB  | VAL | A | 195 | 11.889 | 31.621 | 30.828 | 1.00 | 21.72 | C |
| ATOM | 1452 | CG1 | VAL | A | 195 | 13.038 | 32.476 | 30.327 | 1.00 | 21.84 | C |
| ATOM | 1453 | CG2 | VAL | A | 195 | 10.628 | 31.904 | 30.043 | 1.00 | 23.61 | C |
| ATOM | 1454 | N   | THR | A | 196 | 14.644 | 29.834 | 30.813 | 1.00 | 19.77 | N |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1455 | CA  | THR | A | 196 | 15.980 | 29.917 | 31.376 | 1.00 | 20.37 | C |
| ATOM | 1456 | C   | THR | A | 196 | 16.467 | 31.291 | 30.933 | 1.00 | 20.92 | C |
| ATOM | 1457 | O   | THR | A | 196 | 16.649 | 31.505 | 29.724 | 1.00 | 20.45 | O |
| ATOM | 1458 | CB  | THR | A | 196 | 16.882 | 28.865 | 30.793 | 1.00 | 19.87 | C |
| ATOM | 1459 | OG1 | THR | A | 196 | 16.457 | 27.564 | 31.227 | 1.00 | 21.07 | O |
| ATOM | 1460 | CG2 | THR | A | 196 | 18.273 | 29.043 | 31.340 | 1.00 | 20.00 | C |
| ATOM | 1461 | N   | PRO | A | 197 | 16.602 | 32.225 | 31.879 | 1.00 | 21.53 | N |
| ATOM | 1462 | CA  | PRO | A | 197 | 16.997 | 33.609 | 31.572 | 1.00 | 22.24 | C |
| ATOM | 1463 | C   | PRO | A | 197 | 18.375 | 33.688 | 30.952 | 1.00 | 22.26 | C |
| ATOM | 1464 | O   | PRO | A | 197 | 19.195 | 32.773 | 31.130 | 1.00 | 22.66 | O |
| ATOM | 1465 | CB  | PRO | A | 197 | 16.998 | 34.305 | 32.934 | 1.00 | 22.51 | C |
| ATOM | 1466 | CG  | PRO | A | 197 | 16.282 | 33.411 | 33.839 | 1.00 | 22.92 | C |
| ATOM | 1467 | CD  | PRO | A | 197 | 16.367 | 32.028 | 33.312 | 1.00 | 21.85 | C |
| ATOM | 1468 | N   | ALA | A | 198 | 18.606 | 34.776 | 30.234 | 1.00 | 21.54 | N |
| ATOM | 1469 | CA  | ALA | A | 198 | 19.821 | 34.976 | 29.486 | 1.00 | 21.47 | C |
| ATOM | 1470 | C   | ALA | A | 198 | 21.110 | 34.764 | 30.282 | 1.00 | 21.22 | C |
| ATOM | 1471 | O   | ALA | A | 198 | 21.298 | 35.310 | 31.386 | 1.00 | 20.56 | O |
| ATOM | 1472 | CB  | ALA | A | 198 | 19.809 | 36.397 | 28.891 | 1.00 | 21.92 | C |
| ATOM | 1473 | N   | HIS | A | 199 | 22.023 | 34.020 | 29.683 | 1.00 | 21.01 | N |
| ATOM | 1474 | CA  | HIS | A | 199 | 23.321 | 33.764 | 30.288 | 1.00 | 21.40 | C |
| ATOM | 1475 | C   | HIS | A | 199 | 24.250 | 33.279 | 29.213 | 1.00 | 21.61 | C |
| ATOM | 1476 | O   | HIS | A | 199 | 23.811 | 33.017 | 28.089 | 1.00 | 21.18 | O |
| ATOM | 1477 | CB  | HIS | A | 199 | 23.217 | 32.669 | 31.338 | 1.00 | 21.05 | C |
| ATOM | 1478 | CG  | HIS | A | 199 | 22.864 | 31.354 | 30.746 | 1.00 | 22.98 | C |
| ATOM | 1479 | ND1 | HIS | A | 199 | 21.576 | 31.048 | 30.370 | 1.00 | 21.97 | N |
| ATOM | 1480 | CD2 | HIS | A | 199 | 23.630 | 30.287 | 30.399 | 1.00 | 21.48 | C |
| ATOM | 1481 | CE1 | HIS | A | 199 | 21.558 | 29.838 | 29.838 | 1.00 | 22.85 | C |
| ATOM | 1482 | NE2 | HIS | A | 199 | 22.791 | 29.368 | 29.821 | 1.00 | 24.36 | N |
| ATOM | 1483 | N   | TYR | A | 200 | 25.538 | 33.177 | 29.555 | 1.00 | 22.22 | N |
| ATOM | 1484 | CA  | TYR | A | 200 | 26.531 | 32.597 | 28.654 | 1.00 | 22.56 | C |
| ATOM | 1485 | C   | TYR | A | 200 | 27.234 | 31.448 | 29.380 | 1.00 | 22.96 | C |
| ATOM | 1486 | O   | TYR | A | 200 | 27.293 | 31.430 | 30.612 | 1.00 | 22.90 | O |
| ATOM | 1487 | CB  | TYR | A | 200 | 27.528 | 33.610 | 28.129 | 1.00 | 22.56 | C |
| ATOM | 1488 | CG  | TYR | A | 200 | 28.492 | 34.228 | 29.145 | 1.00 | 23.02 | C |
| ATOM | 1489 | CD1 | TYR | A | 200 | 29.731 | 33.671 | 29.385 | 1.00 | 22.79 | C |
| ATOM | 1490 | CD2 | TYR | A | 200 | 28.180 | 35.419 | 29.799 | 1.00 | 23.89 | C |
| ATOM | 1491 | CE1 | TYR | A | 200 | 30.612 | 34.229 | 30.283 | 1.00 | 22.32 | C |
| ATOM | 1492 | CE2 | TYR | A | 200 | 29.062 | 35.991 | 30.722 | 1.00 | 22.06 | C |
| ATOM | 1493 | CZ  | TYR | A | 200 | 30.277 | 35.402 | 30.947 | 1.00 | 22.13 | C |
| ATOM | 1494 | OH  | TYR | A | 200 | 31.163 | 35.957 | 31.843 | 1.00 | 20.46 | O |
| ATOM | 1495 | N   | ASP | A | 201 | 27.723 | 30.467 | 28.619 | 1.00 | 23.11 | N |
| ATOM | 1496 | CA  | ASP | A | 201 | 28.433 | 29.326 | 29.213 | 1.00 | 23.02 | C |
| ATOM | 1497 | C   | ASP | A | 201 | 29.833 | 29.338 | 28.687 | 1.00 | 23.38 | C |
| ATOM | 1498 | O   | ASP | A | 201 | 30.038 | 29.811 | 27.597 | 1.00 | 24.05 | O |
| ATOM | 1499 | CB  | ASP | A | 201 | 27.776 | 28.012 | 28.829 | 1.00 | 22.85 | C |
| ATOM | 1500 | CG  | ASP | A | 201 | 26.365 | 27.898 | 29.338 | 1.00 | 21.12 | C |
| ATOM | 1501 | OD1 | ASP | A | 201 | 26.176 | 27.802 | 30.568 | 1.00 | 23.22 | O |
| ATOM | 1502 | OD2 | ASP | A | 201 | 25.387 | 27.845 | 28.574 | 1.00 | 20.55 | O |
| ATOM | 1503 | N   | GLU | A | 202 | 30.799 | 28.820 | 29.437 | 1.00 | 23.78 | N |
| ATOM | 1504 | CA  | GLU | A | 202 | 32.184 | 28.782 | 28.950 | 1.00 | 25.14 | C |
| ATOM | 1505 | C   | GLU | A | 202 | 32.524 | 27.467 | 28.269 | 1.00 | 24.96 | C |
| ATOM | 1506 | O   | GLU | A | 202 | 33.657 | 27.001 | 28.394 | 1.00 | 26.76 | O |
| ATOM | 1507 | CB  | GLU | A | 202 | 33.218 | 28.965 | 30.091 | 1.00 | 24.67 | C |
| ATOM | 1508 | CG  | GLU | A | 202 | 33.017 | 30.199 | 30.941 | 1.00 | 27.79 | C |
| ATOM | 1509 | CD  | GLU | A | 202 | 34.089 | 30.312 | 32.025 | 1.00 | 30.13 | C |
| ATOM | 1510 | OE1 | GLU | A | 202 | 34.018 | 29.584 | 33.030 | 1.00 | 32.67 | O |
| ATOM | 1511 | OE2 | GLU | A | 202 | 35.010 | 31.114 | 31.844 | 1.00 | 29.05 | O |
| ATOM | 1512 | N   | GLN | A | 203 | 31.547 | 26.818 | 27.653 | 1.00 | 24.30 | N |
| ATOM | 1513 | CA  | GLN | A | 203 | 31.804 | 25.624 | 26.874 | 1.00 | 23.24 | C |
| ATOM | 1514 | C   | GLN | A | 203 | 31.036 | 25.764 | 25.572 | 1.00 | 22.84 | C |
| ATOM | 1515 | O   | GLN | A | 203 | 30.122 | 26.560 | 25.468 | 1.00 | 23.00 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1516 | CB  | GLN | A | 203 | 31.373 | 24.363 | 27.618 | 1.00 | 23.43 | C |
| ATOM | 1517 | CG  | GLN | A | 203 | 32.256 | 24.031 | 28.826 | 1.00 | 23.66 | C |
| ATOM | 1518 | CD  | GLN | A | 203 | 32.061 | 22.612 | 29.354 | 1.00 | 25.58 | C |
| ATOM | 1519 | OE1 | GLN | A | 203 | 31.915 | 21.661 | 28.582 | 1.00 | 27.85 | O |
| ATOM | 1520 | NE2 | GLN | A | 203 | 32.084 | 22.468 | 30.670 | 1.00 | 25.67 | N |
| ATOM | 1521 | N   | GLN | A | 204 | 31.465 | 25.013 | 24.575 | 1.00 | 22.51 | N |
| ATOM | 1522 | CA  | GLN | A | 204 | 30.791 | 24.910 | 23.299 | 1.00 | 22.51 | C |
| ATOM | 1523 | C   | GLN | A | 204 | 29.626 | 23.980 | 23.504 | 1.00 | 21.70 | C |
| ATOM | 1524 | O   | GLN | A | 204 | 29.737 | 23.026 | 24.255 | 1.00 | 21.24 | O |
| ATOM | 1525 | CB  | GLN | A | 204 | 31.718 | 24.307 | 22.255 | 1.00 | 22.29 | C |
| ATOM | 1526 | CG  | GLN | A | 204 | 33.001 | 25.081 | 22.072 | 1.00 | 22.69 | C |
| ATOM | 1527 | CD  | GLN | A | 204 | 32.820 | 26.346 | 21.259 | 1.00 | 22.39 | C |
| ATOM | 1528 | OE1 | GLN | A | 204 | 31.699 | 26.736 | 20.932 | 1.00 | 19.22 | O |
| ATOM | 1529 | NE2 | GLN | A | 204 | 33.937 | 26.970 | 20.906 | 1.00 | 19.77 | N |
| ATOM | 1530 | N   | ASN | A | 205 | 28.523 | 24.241 | 22.810 | 1.00 | 21.48 | N |
| ATOM | 1531 | CA  | ASN | A | 205 | 27.309 | 23.471 | 23.017 | 1.00 | 21.04 | C |
| ATOM | 1532 | C   | ASN | A | 205 | 26.558 | 23.136 | 21.730 | 1.00 | 21.10 | C |
| ATOM | 1533 | O   | ASN | A | 205 | 26.188 | 24.043 | 20.949 | 1.00 | 20.02 | O |
| ATOM | 1534 | CB  | ASN | A | 205 | 26.401 | 24.322 | 23.920 | 1.00 | 21.70 | C |
| ATOM | 1535 | CG  | ASN | A | 205 | 25.084 | 23.654 | 24.269 | 1.00 | 21.87 | C |
| ATOM | 1536 | OD1 | ASN | A | 205 | 24.732 | 22.577 | 23.775 | 1.00 | 22.07 | O |
| ATOM | 1537 | ND2 | ASN | A | 205 | 24.332 | 24.320 | 25.118 | 1.00 | 19.37 | N |
| ATOM | 1538 | N   | PHE | A | 206 | 26.350 | 21.835 | 21.497 | 1.00 | 20.28 | N |
| ATOM | 1539 | CA  | PHE | A | 206 | 25.372 | 21.414 | 20.523 | 1.00 | 20.14 | C |
| ATOM | 1540 | C   | PHE | A | 206 | 24.141 | 21.030 | 21.323 | 1.00 | 19.94 | C |
| ATOM | 1541 | O   | PHE | A | 206 | 24.164 | 20.052 | 22.065 | 1.00 | 20.71 | O |
| ATOM | 1542 | CB  | PHE | A | 206 | 25.851 | 20.238 | 19.693 | 1.00 | 20.65 | C |
| ATOM | 1543 | CG  | PHE | A | 206 | 26.799 | 20.618 | 18.620 | 1.00 | 20.30 | C |
| ATOM | 1544 | CD1 | PHE | A | 206 | 26.394 | 21.438 | 17.600 | 1.00 | 20.89 | C |
| ATOM | 1545 | CD2 | PHE | A | 206 | 28.101 | 20.168 | 18.642 | 1.00 | 21.26 | C |
| ATOM | 1546 | CE1 | PHE | A | 206 | 27.254 | 21.783 | 16.605 | 1.00 | 22.17 | C |
| ATOM | 1547 | CE2 | PHE | A | 206 | 28.980 | 20.523 | 17.641 | 1.00 | 21.31 | C |
| ATOM | 1548 | CZ  | PHE | A | 206 | 28.558 | 21.336 | 16.632 | 1.00 | 21.79 | C |
| ATOM | 1549 | N   | PHE | A | 207 | 23.058 | 21.764 | 21.081 | 1.00 | 19.87 | N |
| ATOM | 1550 | CA  | PHE | A | 207 | 21.790 | 21.723 | 21.824 | 1.00 | 20.08 | C |
| ATOM | 1551 | C   | PHE | A | 207 | 20.766 | 20.988 | 20.975 | 1.00 | 20.29 | C |
| ATOM | 1552 | O   | PHE | A | 207 | 20.276 | 21.519 | 20.011 | 1.00 | 19.94 | O |
| ATOM | 1553 | CB  | PHE | A | 207 | 21.385 | 23.190 | 22.083 | 1.00 | 20.46 | C |
| ATOM | 1554 | CG  | PHE | A | 207 | 20.129 | 23.404 | 22.890 | 1.00 | 19.14 | C |
| ATOM | 1555 | CD1 | PHE | A | 207 | 18.947 | 23.708 | 22.267 | 1.00 | 19.77 | C |
| ATOM | 1556 | CD2 | PHE | A | 207 | 20.169 | 23.428 | 24.259 | 1.00 | 19.99 | C |
| ATOM | 1557 | CE1 | PHE | A | 207 | 17.818 | 23.980 | 22.984 | 1.00 | 21.67 | C |
| ATOM | 1558 | CE2 | PHE | A | 207 | 19.037 | 23.683 | 24.992 | 1.00 | 22.36 | C |
| ATOM | 1559 | CZ  | PHE | A | 207 | 17.854 | 23.975 | 24.351 | 1.00 | 22.30 | C |
| ATOM | 1560 | N   | ALA | A | 208 | 20.480 | 19.746 | 21.352 | 1.00 | 21.01 | N |
| ATOM | 1561 | CA  | ALA | A | 208 | 19.688 | 18.827 | 20.541 | 1.00 | 21.26 | C |
| ATOM | 1562 | C   | ALA | A | 208 | 18.260 | 18.669 | 21.030 | 1.00 | 21.74 | C |
| ATOM | 1563 | O   | ALA | A | 208 | 18.000 | 17.983 | 22.049 | 1.00 | 21.21 | O |
| ATOM | 1564 | CB  | ALA | A | 208 | 20.365 | 17.464 | 20.557 | 1.00 | 20.94 | C |
| ATOM | 1565 | N   | GLN | A | 209 | 17.329 | 19.245 | 20.276 | 1.00 | 21.56 | N |
| ATOM | 1566 | CA  | GLN | A | 209 | 15.940 | 19.219 | 20.697 | 1.00 | 21.78 | C |
| ATOM | 1567 | C   | GLN | A | 209 | 15.289 | 17.864 | 20.393 | 1.00 | 21.84 | C |
| ATOM | 1568 | O   | GLN | A | 209 | 15.506 | 17.245 | 19.323 | 1.00 | 20.40 | O |
| ATOM | 1569 | CB  | GLN | A | 209 | 15.203 | 20.391 | 20.068 | 1.00 | 22.08 | C |
| ATOM | 1570 | CG  | GLN | A | 209 | 13.790 | 20.597 | 20.542 | 1.00 | 22.02 | C |
| ATOM | 1571 | CD  | GLN | A | 209 | 13.688 | 20.986 | 22.013 | 1.00 | 22.84 | C |
| ATOM | 1572 | OE1 | GLN | A | 209 | 14.700 | 21.240 | 22.678 | 1.00 | 22.55 | O |
| ATOM | 1573 | NE2 | GLN | A | 209 | 12.448 | 21.034 | 22.524 | 1.00 | 21.97 | N |
| ATOM | 1574 | N   | ILE | A | 210 | 14.480 | 17.418 | 21.351 | 1.00 | 22.17 | N |
| ATOM | 1575 | CA  | ILE | A | 210 | 13.904 | 16.084 | 21.329 | 1.00 | 22.53 | C |
| ATOM | 1576 | C   | ILE | A | 210 | 12.397 | 16.074 | 21.316 | 1.00 | 23.45 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1577 | O   | ILE | A | 210 | 11.813 | 15.429 | 20.467 | 1.00 | 24.08 | O |
| ATOM | 1578 | CB  | ILE | A | 210 | 14.411 | 15.306 | 22.541 | 1.00 | 22.81 | C |
| ATOM | 1579 | CG1 | ILE | A | 210 | 15.857 | 14.886 | 22.284 | 1.00 | 23.77 | C |
| ATOM | 1580 | CG2 | ILE | A | 210 | 13.573 | 14.064 | 22.785 | 1.00 | 23.17 | C |
| ATOM | 1581 | CD1 | ILE | A | 210 | 16.631 | 14.512 | 23.519 | 1.00 | 24.86 | C |
| ATOM | 1582 | N   | LYS | A | 211 | 11.772 | 16.778 | 22.258 | 1.00 | 23.73 | N |
| ATOM | 1583 | CA  | LYS | A | 211 | 10.318 | 16.829 | 22.351 | 1.00 | 22.99 | C |
| ATOM | 1584 | C   | LYS | A | 211 | 9.873  | 18.253 | 22.566 | 1.00 | 22.73 | C |
| ATOM | 1585 | O   | LYS | A | 211 | 10.436 | 18.969 | 23.391 | 1.00 | 22.34 | O |
| ATOM | 1586 | CB  | LYS | A | 211 | 9.818  | 16.014 | 23.527 | 1.00 | 23.40 | C |
| ATOM | 1587 | CG  | LYS | A | 211 | 8.285  | 15.757 | 23.509 | 1.00 | 24.55 | C |
| ATOM | 1588 | CD  | LYS | A | 211 | 7.794  | 15.232 | 24.870 | 1.00 | 25.75 | C |
| ATOM | 1589 | CE  | LYS | A | 211 | 6.389  | 14.579 | 24.861 | 1.00 | 25.61 | C |
| ATOM | 1590 | NZ  | LYS | A | 211 | 5.580  | 14.641 | 23.613 | 1.00 | 25.29 | N |
| ATOM | 1591 | N   | GLY | A | 212 | 8.832  | 18.655 | 21.847 | 1.00 | 22.34 | N |
| ATOM | 1592 | CA  | GLY | A | 212 | 8.292  | 19.989 | 21.983 | 1.00 | 22.46 | C |
| ATOM | 1593 | C   | GLY | A | 212 | 9.188  | 21.026 | 21.338 | 1.00 | 22.40 | C |
| ATOM | 1594 | O   | GLY | A | 212 | 10.172 | 20.705 | 20.650 | 1.00 | 21.93 | O |
| ATOM | 1595 | N   | TYR | A | 213 | 8.859  | 22.281 | 21.592 | 1.00 | 22.95 | N |
| ATOM | 1596 | CA  | TYR | A | 213 | 9.530  | 23.400 | 20.944 | 1.00 | 23.32 | C |
| ATOM | 1597 | C   | TYR | A | 213 | 10.079 | 24.412 | 21.926 | 1.00 | 23.27 | C |
| ATOM | 1598 | O   | TYR | A | 213 | 9.434  | 24.740 | 22.918 | 1.00 | 23.34 | O |
| ATOM | 1599 | CB  | TYR | A | 213 | 8.547  | 24.092 | 20.012 | 1.00 | 23.77 | C |
| ATOM | 1600 | CG  | TYR | A | 213 | 8.133  | 23.198 | 18.887 | 1.00 | 25.58 | C |
| ATOM | 1601 | CD1 | TYR | A | 213 | 7.110  | 22.261 | 19.041 | 1.00 | 28.74 | C |
| ATOM | 1602 | CD2 | TYR | A | 213 | 8.798  | 23.253 | 17.687 | 1.00 | 28.55 | C |
| ATOM | 1603 | CE1 | TYR | A | 213 | 6.764  | 21.410 | 17.995 | 1.00 | 30.77 | C |
| ATOM | 1604 | CE2 | TYR | A | 213 | 8.465  | 22.429 | 16.651 | 1.00 | 30.41 | C |
| ATOM | 1605 | CZ  | TYR | A | 213 | 7.461  | 21.516 | 16.795 | 1.00 | 31.44 | C |
| ATOM | 1606 | OH  | TYR | A | 213 | 7.188  | 20.720 | 15.708 | 1.00 | 35.50 | O |
| ATOM | 1607 | N   | LYS | A | 214 | 11.270 | 24.911 | 21.620 | 1.00 | 22.60 | N |
| ATOM | 1608 | CA  | LYS | A | 214 | 11.916 | 25.911 | 22.431 | 1.00 | 22.58 | C |
| ATOM | 1609 | C   | LYS | A | 214 | 12.353 | 27.077 | 21.576 | 1.00 | 22.52 | C |
| ATOM | 1610 | O   | LYS | A | 214 | 12.937 | 26.898 | 20.493 | 1.00 | 23.74 | O |
| ATOM | 1611 | CB  | LYS | A | 214 | 13.132 | 25.345 | 23.169 | 1.00 | 22.31 | C |
| ATOM | 1612 | CG  | LYS | A | 214 | 12.784 | 24.539 | 24.392 | 1.00 | 22.79 | C |
| ATOM | 1613 | CD  | LYS | A | 214 | 14.053 | 24.007 | 25.077 | 1.00 | 22.96 | C |
| ATOM | 1614 | CE  | LYS | A | 214 | 13.821 | 23.675 | 26.530 | 1.00 | 20.69 | C |
| ATOM | 1615 | NZ  | LYS | A | 214 | 15.076 | 23.085 | 27.149 | 1.00 | 19.14 | N |
| ATOM | 1616 | N   | ARG | A | 215 | 12.037 | 28.277 | 22.047 | 1.00 | 21.95 | N |
| ATOM | 1617 | CA  | ARG | A | 215 | 12.480 | 29.482 | 21.378 | 1.00 | 21.48 | C |
| ATOM | 1618 | C   | ARG | A | 215 | 13.790 | 29.864 | 22.018 | 1.00 | 21.06 | C |
| ATOM | 1619 | O   | ARG | A | 215 | 13.890 | 29.954 | 23.230 | 1.00 | 20.53 | O |
| ATOM | 1620 | CB  | ARG | A | 215 | 11.466 | 30.582 | 21.576 | 1.00 | 22.15 | C |
| ATOM | 1621 | CG  | ARG | A | 215 | 11.843 | 31.913 | 20.969 | 1.00 | 22.00 | C |
| ATOM | 1622 | CD  | ARG | A | 215 | 11.231 | 33.041 | 21.727 | 1.00 | 23.87 | C |
| ATOM | 1623 | NE  | ARG | A | 215 | 11.224 | 34.272 | 20.959 | 1.00 | 25.87 | N |
| ATOM | 1624 | CZ  | ARG | A | 215 | 10.566 | 35.364 | 21.297 | 1.00 | 25.54 | C |
| ATOM | 1625 | NH1 | ARG | A | 215 | 9.873  | 35.425 | 22.423 | 1.00 | 24.05 | N |
| ATOM | 1626 | NH2 | ARG | A | 215 | 10.634 | 36.420 | 20.505 | 1.00 | 29.37 | N |
| ATOM | 1627 | N   | CYS | A | 216 | 14.794 | 30.090 | 21.193 | 1.00 | 21.48 | N |
| ATOM | 1628 | CA  | CYS | A | 216 | 16.123 | 30.355 | 21.668 | 1.00 | 21.40 | C |
| ATOM | 1629 | C   | CYS | A | 216 | 16.533 | 31.723 | 21.146 | 1.00 | 21.86 | C |
| ATOM | 1630 | O   | CYS | A | 216 | 16.532 | 31.952 | 19.948 | 1.00 | 22.82 | O |
| ATOM | 1631 | CB  | CYS | A | 216 | 17.079 | 29.309 | 21.127 | 1.00 | 21.46 | C |
| ATOM | 1632 | SG  | CYS | A | 216 | 16.689 | 27.562 | 21.469 | 1.00 | 22.63 | S |
| ATOM | 1633 | N   | ILE | A | 217 | 16.878 | 32.630 | 22.045 | 1.00 | 21.29 | N |
| ATOM | 1634 | CA  | ILE | A | 217 | 17.331 | 33.960 | 21.663 | 1.00 | 21.28 | C |
| ATOM | 1635 | C   | ILE | A | 217 | 18.782 | 34.114 | 22.102 | 1.00 | 20.86 | C |
| ATOM | 1636 | O   | ILE | A | 217 | 19.085 | 34.007 | 23.310 | 1.00 | 21.04 | O |
| ATOM | 1637 | CB  | ILE | A | 217 | 16.456 | 35.025 | 22.327 | 1.00 | 21.80 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1638 | CG1 | ILE | A | 217 | 14.978 | 34.807 | 21.955 | 1.00 | 22.90 | C |
| ATOM | 1639 | CG2 | ILE | A | 217 | 16.874 | 36.414 | 21.861 | 1.00 | 22.72 | C |
| ATOM | 1640 | CD1 | ILE | A | 217 | 14.031 | 35.695 | 22.693 | 1.00 | 24.99 | C |
| ATOM | 1641 | N   | LEU | A | 218 | 19.666 | 34.346 | 21.128 | 1.00 | 20.25 | N |
| ATOM | 1642 | CA  | LEU | A | 218 | 21.094 | 34.451 | 21.373 | 1.00 | 20.55 | C |
| ATOM | 1643 | C   | LEU | A | 218 | 21.630 | 35.853 | 21.128 | 1.00 | 21.19 | C |
| ATOM | 1644 | O   | LEU | A | 218 | 21.141 | 36.560 | 20.253 | 1.00 | 21.62 | O |
| ATOM | 1645 | CB  | LEU | A | 218 | 21.874 | 33.493 | 20.467 | 1.00 | 20.31 | C |
| ATOM | 1646 | CG  | LEU | A | 218 | 21.964 | 32.019 | 20.906 | 1.00 | 20.46 | C |
| ATOM | 1647 | CD1 | LEU | A | 218 | 20.628 | 31.415 | 21.054 | 1.00 | 20.19 | C |
| ATOM | 1648 | CD2 | LEU | A | 218 | 22.732 | 31.229 | 19.907 | 1.00 | 22.84 | C |
| ATOM | 1649 | N   | PHE | A | 219 | 22.658 | 36.231 | 21.886 | 1.00 | 21.06 | N |
| ATOM | 1650 | CA  | PHE | A | 219 | 23.331 | 37.498 | 21.682 | 1.00 | 21.62 | C |
| ATOM | 1651 | C   | PHE | A | 219 | 24.842 | 37.244 | 21.611 | 1.00 | 21.87 | C |
| ATOM | 1652 | O   | PHE | A | 219 | 25.390 | 36.490 | 22.416 | 1.00 | 21.88 | O |
| ATOM | 1653 | CB  | PHE | A | 219 | 23.005 | 38.484 | 22.820 | 1.00 | 20.94 | C |
| ATOM | 1654 | CG  | PHE | A | 219 | 21.541 | 38.617 | 23.106 | 1.00 | 21.13 | C |
| ATOM | 1655 | CD1 | PHE | A | 219 | 20.907 | 37.779 | 23.995 | 1.00 | 21.92 | C |
| ATOM | 1656 | CD2 | PHE | A | 219 | 20.785 | 39.589 | 22.476 | 1.00 | 24.21 | C |
| ATOM | 1657 | CE1 | PHE | A | 219 | 19.563 | 37.915 | 24.250 | 1.00 | 21.95 | C |
| ATOM | 1658 | CE2 | PHE | A | 219 | 19.442 | 39.724 | 22.735 | 1.00 | 22.06 | C |
| ATOM | 1659 | CZ  | PHE | A | 219 | 18.840 | 38.904 | 23.621 | 1.00 | 23.11 | C |
| ATOM | 1660 | N   | PRO | A | 220 | 25.512 | 37.877 | 20.662 | 1.00 | 22.38 | N |
| ATOM | 1661 | CA  | PRO | A | 220 | 26.962 | 37.744 | 20.557 | 1.00 | 22.81 | C |
| ATOM | 1662 | C   | PRO | A | 220 | 27.683 | 38.287 | 21.793 | 1.00 | 22.78 | C |
| ATOM | 1663 | O   | PRO | A | 220 | 27.173 | 39.123 | 22.564 | 1.00 | 22.88 | O |
| ATOM | 1664 | CB  | PRO | A | 220 | 27.335 | 38.561 | 19.317 | 1.00 | 22.81 | C |
| ATOM | 1665 | CG  | PRO | A | 220 | 26.005 | 39.005 | 18.685 | 1.00 | 23.68 | C |
| ATOM | 1666 | CD  | PRO | A | 220 | 24.940 | 38.792 | 19.663 | 1.00 | 22.86 | C |
| ATOM | 1667 | N   | PRO | A | 221 | 28.885 | 37.774 | 21.999 | 1.00 | 22.84 | N |
| ATOM | 1668 | CA  | PRO | A | 221 | 29.724 | 38.204 | 23.124 | 1.00 | 22.73 | C |
| ATOM | 1669 | C   | PRO | A | 221 | 29.976 | 39.714 | 23.143 | 1.00 | 22.28 | C |
| ATOM | 1670 | O   | PRO | A | 221 | 30.192 | 40.279 | 24.212 | 1.00 | 21.03 | O |
| ATOM | 1671 | CB  | PRO | A | 221 | 31.030 | 37.455 | 22.892 | 1.00 | 22.78 | C |
| ATOM | 1672 | CG  | PRO | A | 221 | 30.644 | 36.296 | 22.026 | 1.00 | 23.22 | C |
| ATOM | 1673 | CD  | PRO | A | 221 | 29.521 | 36.733 | 21.174 | 1.00 | 22.58 | C |
| ATOM | 1674 | N   | ASP | A | 222 | 29.897 | 40.378 | 21.993 | 1.00 | 22.60 | N |
| ATOM | 1675 | CA  | ASP | A | 222 | 30.172 | 41.821 | 21.965 | 1.00 | 22.84 | C |
| ATOM | 1676 | C   | ASP | A | 222 | 28.996 | 42.623 | 22.493 | 1.00 | 23.36 | C |
| ATOM | 1677 | O   | ASP | A | 222 | 29.031 | 43.847 | 22.500 | 1.00 | 24.43 | O |
| ATOM | 1678 | CB  | ASP | A | 222 | 30.638 | 42.308 | 20.579 | 1.00 | 22.47 | C |
| ATOM | 1679 | CG  | ASP | A | 222 | 29.502 | 42.389 | 19.537 | 1.00 | 25.07 | C |
| ATOM | 1680 | OD1 | ASP | A | 222 | 28.355 | 41.942 | 19.764 | 1.00 | 25.24 | O |
| ATOM | 1681 | OD2 | ASP | A | 222 | 29.690 | 42.876 | 18.410 | 1.00 | 29.46 | O |
| ATOM | 1682 | N   | GLN | A | 223 | 27.940 | 41.940 | 22.926 | 1.00 | 23.79 | N |
| ATOM | 1683 | CA  | GLN | A | 223 | 26.826 | 42.624 | 23.565 | 1.00 | 23.85 | C |
| ATOM | 1684 | C   | GLN | A | 223 | 26.942 | 42.570 | 25.114 | 1.00 | 23.37 | C |
| ATOM | 1685 | O   | GLN | A | 223 | 25.986 | 42.875 | 25.850 | 1.00 | 23.78 | O |
| ATOM | 1686 | CB  | GLN | A | 223 | 25.510 | 42.084 | 23.007 | 1.00 | 24.80 | C |
| ATOM | 1687 | CG  | GLN | A | 223 | 25.217 | 42.672 | 21.550 | 1.00 | 28.46 | C |
| ATOM | 1688 | CD  | GLN | A | 223 | 23.786 | 42.471 | 21.094 | 1.00 | 32.35 | C |
| ATOM | 1689 | OE1 | GLN | A | 223 | 22.861 | 42.619 | 21.893 | 1.00 | 36.73 | O |
| ATOM | 1690 | NE2 | GLN | A | 223 | 23.592 | 42.105 | 19.815 | 1.00 | 33.48 | N |
| ATOM | 1691 | N   | PHE | A | 224 | 28.111 | 42.167 | 25.601 | 1.00 | 21.59 | N |
| ATOM | 1692 | CA  | PHE | A | 224 | 28.394 | 42.195 | 27.035 | 1.00 | 21.84 | C |
| ATOM | 1693 | C   | PHE | A | 224 | 27.888 | 43.509 | 27.706 | 1.00 | 21.56 | C |
| ATOM | 1694 | O   | PHE | A | 224 | 27.233 | 43.455 | 28.738 | 1.00 | 20.27 | O |
| ATOM | 1695 | CB  | PHE | A | 224 | 29.917 | 42.068 | 27.271 | 1.00 | 21.34 | C |
| ATOM | 1696 | CG  | PHE | A | 224 | 30.309 | 41.943 | 28.732 | 1.00 | 22.22 | C |
| ATOM | 1697 | CD1 | PHE | A | 224 | 30.449 | 43.071 | 29.540 | 1.00 | 21.80 | C |
| ATOM | 1698 | CD2 | PHE | A | 224 | 30.583 | 40.723 | 29.279 | 1.00 | 20.92 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1699 | CE1 | PHE | A | 224 | 30.842 | 42.945 | 30.868 | 1.00 | 22.58 | C |
| ATOM | 1700 | CE2 | PHE | A | 224 | 30.979 | 40.593 | 30.587 | 1.00 | 22.14 | C |
| ATOM | 1701 | CZ  | PHE | A | 224 | 31.087 | 41.725 | 31.394 | 1.00 | 22.16 | C |
| ATOM | 1702 | N   | GLU | A | 225 | 28.190 | 44.665 | 27.106 | 1.00 | 22.03 | N |
| ATOM | 1703 | CA  | GLU | A | 225 | 27.813 | 45.963 | 27.677 | 1.00 | 23.55 | C |
| ATOM | 1704 | C   | GLU | A | 225 | 26.322 | 46.216 | 27.764 | 1.00 | 23.06 | C |
| ATOM | 1705 | O   | GLU | A | 225 | 25.907 | 47.129 | 28.483 | 1.00 | 22.10 | O |
| ATOM | 1706 | CB  | GLU | A | 225 | 28.396 | 47.111 | 26.856 | 1.00 | 24.92 | C |
| ATOM | 1707 | CG  | GLU | A | 225 | 29.897 | 47.228 | 27.013 | 1.00 | 30.17 | C |
| ATOM | 1708 | CD  | GLU | A | 225 | 30.386 | 48.632 | 27.280 | 1.00 | 36.52 | C |
| ATOM | 1709 | OE1 | GLU | A | 225 | 29.901 | 49.319 | 28.242 | 1.00 | 40.52 | O |
| ATOM | 1710 | OE2 | GLU | A | 225 | 31.310 | 49.028 | 26.532 | 1.00 | 41.63 | O |
| ATOM | 1711 | N   | CYS | A | 226 | 25.532 | 45.456 | 27.003 | 1.00 | 22.07 | N |
| ATOM | 1712 | CA  | CYS | A | 226 | 24.087 | 45.619 | 27.027 | 1.00 | 22.09 | C |
| ATOM | 1713 | C   | CYS | A | 226 | 23.372 | 44.631 | 27.935 | 1.00 | 21.89 | C |
| ATOM | 1714 | O   | CYS | A | 226 | 22.170 | 44.781 | 28.162 | 1.00 | 20.73 | O |
| ATOM | 1715 | CB  | CYS | A | 226 | 23.523 | 45.416 | 25.630 | 1.00 | 22.22 | C |
| ATOM | 1716 | SG  | CYS | A | 226 | 24.206 | 46.488 | 24.368 | 1.00 | 22.59 | S |
| ATOM | 1717 | N   | LEU | A | 227 | 24.102 | 43.633 | 28.451 | 1.00 | 22.08 | N |
| ATOM | 1718 | CA  | LEU | A | 227 | 23.467 | 42.529 | 29.169 | 1.00 | 22.08 | C |
| ATOM | 1719 | C   | LEU | A | 227 | 23.771 | 42.393 | 30.657 | 1.00 | 21.99 | C |
| ATOM | 1720 | O   | LEU | A | 227 | 23.118 | 41.611 | 31.373 | 1.00 | 22.28 | O |
| ATOM | 1721 | CB  | LEU | A | 227 | 23.751 | 41.244 | 28.418 | 1.00 | 22.29 | C |
| ATOM | 1722 | CG  | LEU | A | 227 | 22.874 | 41.185 | 27.158 | 1.00 | 23.54 | C |
| ATOM | 1723 | CD1 | LEU | A | 227 | 23.428 | 40.186 | 26.144 | 1.00 | 23.51 | C |
| ATOM | 1724 | CD2 | LEU | A | 227 | 21.423 | 40.819 | 27.544 | 1.00 | 24.49 | C |
| ATOM | 1725 | N   | TYR | A | 228 | 24.763 | 43.140 | 31.109 | 1.00 | 20.87 | N |
| ATOM | 1726 | CA  | TYR | A | 228 | 24.996 | 43.320 | 32.521 | 1.00 | 21.33 | C |
| ATOM | 1727 | C   | TYR | A | 228 | 25.018 | 42.057 | 33.382 | 1.00 | 21.27 | C |
| ATOM | 1728 | O   | TYR | A | 228 | 24.205 | 41.920 | 34.301 | 1.00 | 21.72 | O |
| ATOM | 1729 | CB  | TYR | A | 228 | 23.957 | 44.311 | 33.077 | 1.00 | 20.92 | C |
| ATOM | 1730 | CG  | TYR | A | 228 | 23.949 | 45.649 | 32.339 | 1.00 | 20.91 | C |
| ATOM | 1731 | CD1 | TYR | A | 228 | 24.768 | 46.677 | 32.739 | 1.00 | 18.87 | C |
| ATOM | 1732 | CD2 | TYR | A | 228 | 23.122 | 45.862 | 31.232 | 1.00 | 20.51 | C |
| ATOM | 1733 | CE1 | TYR | A | 228 | 24.780 | 47.912 | 32.076 | 1.00 | 20.36 | C |
| ATOM | 1734 | CE2 | TYR | A | 228 | 23.117 | 47.074 | 30.561 | 1.00 | 21.07 | C |
| ATOM | 1735 | CZ  | TYR | A | 228 | 23.931 | 48.113 | 31.000 | 1.00 | 20.84 | C |
| ATOM | 1736 | OH  | TYR | A | 228 | 23.947 | 49.325 | 30.336 | 1.00 | 19.16 | O |
| ATOM | 1737 | N   | PRO | A | 229 | 25.985 | 41.175 | 33.141 | 1.00 | 20.77 | N |
| ATOM | 1738 | CA  | PRO | A | 229 | 26.128 | 39.971 | 33.966 | 1.00 | 21.05 | C |
| ATOM | 1739 | C   | PRO | A | 229 | 26.428 | 40.332 | 35.408 | 1.00 | 20.08 | C |
| ATOM | 1740 | O   | PRO | A | 229 | 27.021 | 41.379 | 35.675 | 1.00 | 20.20 | O |
| ATOM | 1741 | CB  | PRO | A | 229 | 27.360 | 39.271 | 33.363 | 1.00 | 20.51 | C |
| ATOM | 1742 | CG  | PRO | A | 229 | 28.084 | 40.340 | 32.651 | 1.00 | 21.64 | C |
| ATOM | 1743 | CD  | PRO | A | 229 | 27.025 | 41.241 | 32.105 | 1.00 | 20.97 | C |
| ATOM | 1744 | N   | TYR | A | 230 | 25.988 | 39.490 | 36.326 | 1.00 | 19.73 | N |
| ATOM | 1745 | CA  | TYR | A | 230 | 26.282 | 39.656 | 37.724 | 1.00 | 18.80 | C |
| ATOM | 1746 | C   | TYR | A | 230 | 27.809 | 39.657 | 37.947 | 1.00 | 18.61 | C |
| ATOM | 1747 | O   | TYR | A | 230 | 28.575 | 39.250 | 37.094 | 1.00 | 18.26 | O |
| ATOM | 1748 | CB  | TYR | A | 230 | 25.669 | 38.507 | 38.520 | 1.00 | 18.86 | C |
| ATOM | 1749 | CG  | TYR | A | 230 | 24.172 | 38.597 | 38.725 | 1.00 | 19.28 | C |
| ATOM | 1750 | CD1 | TYR | A | 230 | 23.297 | 38.110 | 37.760 | 1.00 | 18.53 | C |
| ATOM | 1751 | CD2 | TYR | A | 230 | 23.629 | 39.172 | 39.885 | 1.00 | 19.38 | C |
| ATOM | 1752 | CE1 | TYR | A | 230 | 21.932 | 38.161 | 37.935 | 1.00 | 18.86 | C |
| ATOM | 1753 | CE2 | TYR | A | 230 | 22.234 | 39.222 | 40.076 | 1.00 | 19.53 | C |
| ATOM | 1754 | CZ  | TYR | A | 230 | 21.404 | 38.719 | 39.073 | 1.00 | 20.93 | C |
| ATOM | 1755 | OH  | TYR | A | 230 | 20.034 | 38.771 | 39.176 | 1.00 | 23.69 | O |
| ATOM | 1756 | N   | PRO | A | 231 | 28.251 | 40.137 | 39.098 | 1.00 | 18.40 | N |
| ATOM | 1757 | CA  | PRO | A | 231 | 29.651 | 39.983 | 39.476 | 1.00 | 18.58 | C |
| ATOM | 1758 | C   | PRO | A | 231 | 30.070 | 38.507 | 39.399 | 1.00 | 19.41 | C |
| ATOM | 1759 | O   | PRO | A | 231 | 29.240 | 37.624 | 39.654 | 1.00 | 18.89 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1760 | CB  | PRO | A | 231 | 29.675 | 40.477 | 40.931 | 1.00 | 18.95 | C |
| ATOM | 1761 | CG  | PRO | A | 231 | 28.542 | 41.507 | 41.001 | 1.00 | 19.02 | C |
| ATOM | 1762 | CD  | PRO | A | 231 | 27.460 | 40.868 | 40.105 | 1.00 | 18.02 | C |
| ATOM | 1763 | N   | VAL | A | 232 | 31.335 | 38.248 | 39.071 | 1.00 | 19.55 | N |
| ATOM | 1764 | CA  | VAL | A | 232 | 31.826 | 36.884 | 38.969 | 1.00 | 20.65 | C |
| ATOM | 1765 | C   | VAL | A | 232 | 31.640 | 36.034 | 40.236 | 1.00 | 20.79 | C |
| ATOM | 1766 | O   | VAL | A | 232 | 31.379 | 34.838 | 40.145 | 1.00 | 21.82 | O |
| ATOM | 1767 | CB  | VAL | A | 232 | 33.318 | 36.869 | 38.545 | 1.00 | 20.71 | C |
| ATOM | 1768 | CG1 | VAL | A | 232 | 33.945 | 35.524 | 38.807 | 1.00 | 21.96 | C |
| ATOM | 1769 | CG2 | VAL | A | 232 | 33.452 | 37.225 | 37.075 | 1.00 | 20.83 | C |
| ATOM | 1770 | N   | HIS | A | 233 | 31.770 | 36.639 | 41.409 | 1.00 | 20.87 | N |
| ATOM | 1771 | CA  | HIS | A | 233 | 31.643 | 35.907 | 42.661 | 1.00 | 20.70 | C |
| ATOM | 1772 | C   | HIS | A | 233 | 30.203 | 35.739 | 43.168 | 1.00 | 20.59 | C |
| ATOM | 1773 | O   | HIS | A | 233 | 29.940 | 35.010 | 44.119 | 1.00 | 20.49 | O |
| ATOM | 1774 | CB  | HIS | A | 233 | 32.482 | 36.593 | 43.706 | 1.00 | 20.63 | C |
| ATOM | 1775 | CG  | HIS | A | 233 | 33.948 | 36.529 | 43.426 | 1.00 | 21.92 | C |
| ATOM | 1776 | ND1 | HIS | A | 233 | 34.659 | 37.595 | 42.913 | 1.00 | 22.17 | N |
| ATOM | 1777 | CD2 | HIS | A | 233 | 34.843 | 35.527 | 43.610 | 1.00 | 22.03 | C |
| ATOM | 1778 | CE1 | HIS | A | 233 | 35.929 | 37.249 | 42.793 | 1.00 | 23.69 | C |
| ATOM | 1779 | NE2 | HIS | A | 233 | 36.066 | 35.998 | 43.203 | 1.00 | 23.04 | N |
| ATOM | 1780 | N   | HIS | A | 234 | 29.273 | 36.433 | 42.543 | 1.00 | 20.53 | N |
| ATOM | 1781 | CA  | HIS | A | 234 | 27.869 | 36.251 | 42.857 | 1.00 | 20.60 | C |
| ATOM | 1782 | C   | HIS | A | 234 | 27.388 | 34.895 | 42.306 | 1.00 | 20.45 | C |
| ATOM | 1783 | O   | HIS | A | 234 | 27.873 | 34.428 | 41.291 | 1.00 | 19.86 | O |
| ATOM | 1784 | CB  | HIS | A | 234 | 27.088 | 37.359 | 42.206 | 1.00 | 20.65 | C |
| ATOM | 1785 | CG  | HIS | A | 234 | 25.661 | 37.441 | 42.625 | 1.00 | 20.68 | C |
| ATOM | 1786 | ND1 | HIS | A | 234 | 24.667 | 36.700 | 42.021 | 1.00 | 21.46 | N |
| ATOM | 1787 | CD2 | HIS | A | 234 | 25.044 | 38.249 | 43.518 | 1.00 | 20.20 | C |
| ATOM | 1788 | CE1 | HIS | A | 234 | 23.504 | 37.013 | 42.563 | 1.00 | 21.99 | C |
| ATOM | 1789 | NE2 | HIS | A | 234 | 23.707 | 37.951 | 43.473 | 1.00 | 21.29 | N |
| ATOM | 1790 | N   | PRO | A | 235 | 26.463 | 34.261 | 43.007 | 1.00 | 20.40 | N |
| ATOM | 1791 | CA  | PRO | A | 235 | 25.888 | 32.993 | 42.572 | 1.00 | 20.85 | C |
| ATOM | 1792 | C   | PRO | A | 235 | 25.360 | 33.021 | 41.152 | 1.00 | 21.20 | C |
| ATOM | 1793 | O   | PRO | A | 235 | 25.437 | 31.984 | 40.502 | 1.00 | 20.43 | O |
| ATOM | 1794 | CB  | PRO | A | 235 | 24.756 | 32.771 | 43.575 | 1.00 | 21.58 | C |
| ATOM | 1795 | CG  | PRO | A | 235 | 25.273 | 33.452 | 44.826 | 1.00 | 20.78 | C |
| ATOM | 1796 | CD  | PRO | A | 235 | 25.941 | 34.685 | 44.317 | 1.00 | 20.56 | C |
| ATOM | 1797 | N   | CYS | A | 236 | 24.905 | 34.173 | 40.663 | 1.00 | 20.46 | N |
| ATOM | 1798 | CA  | CYS | A | 236 | 24.379 | 34.235 | 39.308 | 1.00 | 20.63 | C |
| ATOM | 1799 | C   | CYS | A | 236 | 25.430 | 34.707 | 38.301 | 1.00 | 20.58 | C |
| ATOM | 1800 | O   | CYS | A | 236 | 25.110 | 35.283 | 37.258 | 1.00 | 21.60 | O |
| ATOM | 1801 | CB  | CYS | A | 236 | 23.114 | 35.084 | 39.268 | 1.00 | 20.06 | C |
| ATOM | 1802 | SG  | CYS | A | 236 | 21.824 | 34.377 | 40.326 | 1.00 | 21.70 | S |
| ATOM | 1803 | N   | ASP | A | 237 | 26.693 | 34.474 | 38.629 | 1.00 | 20.17 | N |
| ATOM | 1804 | CA  | ASP | A | 237 | 27.785 | 34.632 | 37.679 | 1.00 | 19.98 | C |
| ATOM | 1805 | C   | ASP | A | 237 | 27.381 | 34.050 | 36.313 | 1.00 | 19.79 | C |
| ATOM | 1806 | O   | ASP | A | 237 | 26.830 | 32.950 | 36.234 | 1.00 | 19.19 | O |
| ATOM | 1807 | CB  | ASP | A | 237 | 28.997 | 33.872 | 38.200 | 1.00 | 19.91 | C |
| ATOM | 1808 | CG  | ASP | A | 237 | 30.209 | 33.968 | 37.290 | 1.00 | 21.43 | C |
| ATOM | 1809 | OD1 | ASP | A | 237 | 30.407 | 35.010 | 36.546 | 1.00 | 18.96 | O |
| ATOM | 1810 | OD2 | ASP | A | 237 | 31.039 | 33.017 | 37.288 | 1.00 | 18.57 | O |
| ATOM | 1811 | N   | ARG | A | 238 | 27.664 | 34.812 | 35.263 | 1.00 | 20.18 | N |
| ATOM | 1812 | CA  | ARG | A | 238 | 27.365 | 34.473 | 33.865 | 1.00 | 21.48 | C |
| ATOM | 1813 | C   | ARG | A | 238 | 25.905 | 34.713 | 33.444 | 1.00 | 20.90 | C |
| ATOM | 1814 | O   | ARG | A | 238 | 25.600 | 34.619 | 32.269 | 1.00 | 21.92 | O |
| ATOM | 1815 | CB  | ARG | A | 238 | 27.765 | 33.024 | 33.531 | 1.00 | 21.70 | C |
| ATOM | 1816 | CG  | ARG | A | 238 | 29.245 | 32.739 | 33.699 | 1.00 | 22.10 | C |
| ATOM | 1817 | CD  | ARG | A | 238 | 29.612 | 31.313 | 33.329 | 1.00 | 23.08 | C |
| ATOM | 1818 | NE  | ARG | A | 238 | 28.988 | 30.409 | 34.278 | 1.00 | 25.97 | N |
| ATOM | 1819 | CZ  | ARG | A | 238 | 27.863 | 29.725 | 34.066 | 1.00 | 27.01 | C |
| ATOM | 1820 | NH1 | ARG | A | 238 | 27.208 | 29.799 | 32.904 | 1.00 | 24.08 | N |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1821 | NH2 | ARG | A | 238 | 27.399 | 28.949 | 35.036 | 1.00 | 27.47 | N |
| ATOM | 1822 | N   | GLN | A | 239 | 25.021 | 35.028 | 34.375 | 1.00 | 20.56 | N |
| ATOM | 1823 | CA  | GLN | A | 239 | 23.641 | 35.334 | 34.014 | 1.00 | 21.11 | C |
| ATOM | 1824 | C   | GLN | A | 239 | 23.459 | 36.865 | 33.920 | 1.00 | 20.84 | C |
| ATOM | 1825 | O   | GLN | A | 239 | 24.145 | 37.624 | 34.610 | 1.00 | 21.25 | O |
| ATOM | 1826 | CB  | GLN | A | 239 | 22.646 | 34.776 | 35.027 | 1.00 | 20.14 | C |
| ATOM | 1827 | CG  | GLN | A | 239 | 23.052 | 33.505 | 35.726 | 1.00 | 22.87 | C |
| ATOM | 1828 | CD  | GLN | A | 239 | 23.281 | 32.320 | 34.807 | 1.00 | 23.97 | C |
| ATOM | 1829 | OE1 | GLN | A | 239 | 22.367 | 31.842 | 34.132 | 1.00 | 23.63 | O |
| ATOM | 1830 | NE2 | GLN | A | 239 | 24.502 | 31.834 | 34.796 | 1.00 | 24.34 | N |
| ATOM | 1831 | N   | SER | A | 240 | 22.541 | 37.307 | 33.071 | 1.00 | 20.31 | N |
| ATOM | 1832 | CA  | SER | A | 240 | 22.246 | 38.725 | 32.926 | 1.00 | 19.92 | C |
| ATOM | 1833 | C   | SER | A | 240 | 21.448 | 39.218 | 34.119 | 1.00 | 20.07 | C |
| ATOM | 1834 | O   | SER | A | 240 | 20.538 | 38.533 | 34.564 | 1.00 | 19.79 | O |
| ATOM | 1835 | CB  | SER | A | 240 | 21.384 | 38.953 | 31.700 | 1.00 | 19.45 | C |
| ATOM | 1836 | OG  | SER | A | 240 | 21.018 | 40.312 | 31.564 | 1.00 | 20.53 | O |
| ATOM | 1837 | N   | GLN | A | 241 | 21.763 | 40.408 | 34.623 | 1.00 | 19.46 | N |
| ATOM | 1838 | CA  | GLN | A | 241 | 20.962 | 40.988 | 35.701 | 1.00 | 20.32 | C |
| ATOM | 1839 | C   | GLN | A | 241 | 19.657 | 41.569 | 35.175 | 1.00 | 20.51 | C |
| ATOM | 1840 | O   | GLN | A | 241 | 18.808 | 41.956 | 35.959 | 1.00 | 21.06 | O |
| ATOM | 1841 | CB  | GLN | A | 241 | 21.697 | 42.141 | 36.417 | 1.00 | 20.15 | C |
| ATOM | 1842 | CG  | GLN | A | 241 | 22.910 | 41.749 | 37.230 | 1.00 | 21.41 | C |
| ATOM | 1843 | CD  | GLN | A | 241 | 23.690 | 42.980 | 37.695 | 1.00 | 22.76 | C |
| ATOM | 1844 | OE1 | GLN | A | 241 | 23.455 | 43.481 | 38.775 | 1.00 | 24.42 | O |
| ATOM | 1845 | NE2 | GLN | A | 241 | 24.585 | 43.465 | 36.871 | 1.00 | 21.93 | N |
| ATOM | 1846 | N   | VAL | A | 242 | 19.489 | 41.678 | 33.862 | 1.00 | 20.66 | N |
| ATOM | 1847 | CA  | VAL | A | 242 | 18.309 | 42.355 | 33.372 | 1.00 | 20.76 | C |
| ATOM | 1848 | C   | VAL | A | 242 | 17.089 | 41.465 | 33.391 | 1.00 | 21.26 | C |
| ATOM | 1849 | O   | VAL | A | 242 | 17.119 | 40.352 | 32.871 | 1.00 | 21.01 | O |
| ATOM | 1850 | CB  | VAL | A | 242 | 18.476 | 42.813 | 31.909 | 1.00 | 20.97 | C |
| ATOM | 1851 | CG1 | VAL | A | 242 | 17.194 | 43.502 | 31.431 | 1.00 | 21.21 | C |
| ATOM | 1852 | CG2 | VAL | A | 242 | 19.687 | 43.704 | 31.716 | 1.00 | 18.95 | C |
| ATOM | 1853 | N   | ASP | A | 243 | 16.001 | 41.960 | 33.958 | 1.00 | 21.16 | N |
| ATOM | 1854 | CA  | ASP | A | 243 | 14.730 | 41.223 | 33.907 | 1.00 | 21.36 | C |
| ATOM | 1855 | C   | ASP | A | 243 | 14.091 | 41.523 | 32.552 | 1.00 | 21.20 | C |
| ATOM | 1856 | O   | ASP | A | 243 | 13.566 | 42.631 | 32.310 | 1.00 | 19.97 | O |
| ATOM | 1857 | CB  | ASP | A | 243 | 13.840 | 41.682 | 35.054 | 1.00 | 21.65 | C |
| ATOM | 1858 | CG  | ASP | A | 243 | 12.474 | 41.051 | 35.037 | 1.00 | 22.45 | C |
| ATOM | 1859 | OD1 | ASP | A | 243 | 12.122 | 40.338 | 34.070 | 1.00 | 25.16 | O |
| ATOM | 1860 | OD2 | ASP | A | 243 | 11.671 | 41.232 | 35.978 | 1.00 | 25.29 | O |
| ATOM | 1861 | N   | PHE | A | 244 | 14.182 | 40.554 | 31.650 | 1.00 | 21.28 | N |
| ATOM | 1862 | CA  | PHE | A | 244 | 13.687 | 40.733 | 30.291 | 1.00 | 21.65 | C |
| ATOM | 1863 | C   | PHE | A | 244 | 12.202 | 41.074 | 30.274 | 1.00 | 22.36 | C |
| ATOM | 1864 | O   | PHE | A | 244 | 11.733 | 41.653 | 29.304 | 1.00 | 22.09 | O |
| ATOM | 1865 | CB  | PHE | A | 244 | 13.915 | 39.478 | 29.442 | 1.00 | 22.22 | C |
| ATOM | 1866 | CG  | PHE | A | 244 | 15.284 | 39.370 | 28.815 | 1.00 | 21.43 | C |
| ATOM | 1867 | CD1 | PHE | A | 244 | 16.414 | 39.800 | 29.465 | 1.00 | 20.12 | C |
| ATOM | 1868 | CD2 | PHE | A | 244 | 15.422 | 38.778 | 27.575 | 1.00 | 21.05 | C |
| ATOM | 1869 | CE1 | PHE | A | 244 | 17.655 | 39.671 | 28.873 | 1.00 | 20.83 | C |
| ATOM | 1870 | CE2 | PHE | A | 244 | 16.645 | 38.643 | 26.993 | 1.00 | 21.47 | C |
| ATOM | 1871 | CZ  | PHE | A | 244 | 17.767 | 39.104 | 27.633 | 1.00 | 20.74 | C |
| ATOM | 1872 | N   | ASP | A | 245 | 11.464 | 40.696 | 31.322 | 1.00 | 23.26 | N |
| ATOM | 1873 | CA  | ASP | A | 245 | 10.035 | 40.973 | 31.393 | 1.00 | 24.31 | C |
| ATOM | 1874 | C   | ASP | A | 245 | 9.756  | 42.401 | 31.877 | 1.00 | 25.05 | C |
| ATOM | 1875 | O   | ASP | A | 245 | 8.679  | 42.916 | 31.646 | 1.00 | 24.27 | O |
| ATOM | 1876 | CB  | ASP | A | 245 | 9.333  | 40.004 | 32.348 | 1.00 | 24.79 | C |
| ATOM | 1877 | CG  | ASP | A | 245 | 9.397  | 38.571 | 31.887 | 1.00 | 25.46 | C |
| ATOM | 1878 | OD1 | ASP | A | 245 | 9.409  | 38.342 | 30.663 | 1.00 | 27.47 | O |
| ATOM | 1879 | OD2 | ASP | A | 245 | 9.445  | 37.610 | 32.678 | 1.00 | 25.22 | O |
| ATOM | 1880 | N   | ASN | A | 246 | 10.702 | 43.006 | 32.589 | 1.00 | 25.30 | N |
| ATOM | 1881 | CA  | ASN | A | 246 | 10.531 | 44.365 | 33.099 | 1.00 | 26.37 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1882 | C   | ASN | A | 246 | 11.876 | 45.054 | 33.204 | 1.00 | 25.61 | C |
| ATOM | 1883 | O   | ASN | A | 246 | 12.436 | 45.192 | 34.282 | 1.00 | 26.05 | O |
| ATOM | 1884 | CB  | ASN | A | 246 | 9.871  | 44.360 | 34.472 | 1.00 | 26.89 | C |
| ATOM | 1885 | CG  | ASN | A | 246 | 9.545  | 45.770 | 34.958 | 1.00 | 30.93 | C |
| ATOM | 1886 | OD1 | ASN | A | 246 | 9.353  | 46.701 | 34.150 | 1.00 | 35.10 | O |
| ATOM | 1887 | ND2 | ASN | A | 246 | 9.493  | 45.943 | 36.281 | 1.00 | 35.04 | N |
| ATOM | 1888 | N   | PRO | A | 247 | 12.415 | 45.450 | 32.068 | 1.00 | 24.71 | N |
| ATOM | 1889 | CA  | PRO | A | 247 | 13.775 | 45.979 | 32.026 | 1.00 | 24.24 | C |
| ATOM | 1890 | C   | PRO | A | 247 | 13.909 | 47.352 | 32.684 | 1.00 | 24.48 | C |
| ATOM | 1891 | O   | PRO | A | 247 | 13.189 | 48.296 | 32.374 | 1.00 | 23.54 | O |
| ATOM | 1892 | CB  | PRO | A | 247 | 14.109 | 46.036 | 30.538 | 1.00 | 24.23 | C |
| ATOM | 1893 | CG  | PRO | A | 247 | 12.900 | 45.524 | 29.803 | 1.00 | 25.13 | C |
| ATOM | 1894 | CD  | PRO | A | 247 | 11.769 | 45.385 | 30.752 | 1.00 | 24.61 | C |
| ATOM | 1895 | N   | ASP | A | 248 | 14.867 | 47.437 | 33.593 | 1.00 | 24.04 | N |
| ATOM | 1896 | CA  | ASP | A | 248 | 15.140 | 48.656 | 34.285 | 1.00 | 24.53 | C |
| ATOM | 1897 | C   | ASP | A | 248 | 16.206 | 49.440 | 33.496 | 1.00 | 24.15 | C |
| ATOM | 1898 | O   | ASP | A | 248 | 17.410 | 49.221 | 33.629 | 1.00 | 23.11 | O |
| ATOM | 1899 | CB  | ASP | A | 248 | 15.609 | 48.312 | 35.689 | 1.00 | 24.75 | C |
| ATOM | 1900 | CG  | ASP | A | 248 | 15.731 | 49.512 | 36.554 | 1.00 | 26.08 | C |
| ATOM | 1901 | OD1 | ASP | A | 248 | 15.956 | 50.616 | 36.009 | 1.00 | 27.08 | O |
| ATOM | 1902 | OD2 | ASP | A | 248 | 15.623 | 49.439 | 37.797 | 1.00 | 30.33 | O |
| ATOM | 1903 | N   | TYR | A | 249 | 15.735 | 50.329 | 32.642 | 1.00 | 24.42 | N |
| ATOM | 1904 | CA  | TYR | A | 249 | 16.612 | 51.129 | 31.807 | 1.00 | 25.30 | C |
| ATOM | 1905 | C   | TYR | A | 249 | 17.462 | 52.136 | 32.589 | 1.00 | 26.13 | C |
| ATOM | 1906 | O   | TYR | A | 249 | 18.495 | 52.584 | 32.083 | 1.00 | 26.46 | O |
| ATOM | 1907 | CB  | TYR | A | 249 | 15.796 | 51.826 | 30.713 | 1.00 | 25.41 | C |
| ATOM | 1908 | CG  | TYR | A | 249 | 15.119 | 50.853 | 29.768 | 1.00 | 22.90 | C |
| ATOM | 1909 | CD1 | TYR | A | 249 | 15.844 | 49.873 | 29.130 | 1.00 | 22.91 | C |
| ATOM | 1910 | CD2 | TYR | A | 249 | 13.760 | 50.923 | 29.519 | 1.00 | 22.21 | C |
| ATOM | 1911 | CE1 | TYR | A | 249 | 15.238 | 48.964 | 28.271 | 1.00 | 22.19 | C |
| ATOM | 1912 | CE2 | TYR | A | 249 | 13.144 | 50.023 | 28.660 | 1.00 | 21.56 | C |
| ATOM | 1913 | CZ  | TYR | A | 249 | 13.895 | 49.044 | 28.046 | 1.00 | 21.23 | C |
| ATOM | 1914 | OH  | TYR | A | 249 | 13.304 | 48.163 | 27.173 | 1.00 | 23.38 | O |
| ATOM | 1915 | N   | GLU | A | 250 | 17.071 | 52.465 | 33.822 | 1.00 | 26.65 | N |
| ATOM | 1916 | CA  | GLU | A | 250 | 17.894 | 53.365 | 34.640 | 1.00 | 27.47 | C |
| ATOM | 1917 | C   | GLU | A | 250 | 19.161 | 52.651 | 35.086 | 1.00 | 26.52 | C |
| ATOM | 1918 | O   | GLU | A | 250 | 20.238 | 53.224 | 35.086 | 1.00 | 27.17 | O |
| ATOM | 1919 | CB  | GLU | A | 250 | 17.133 | 53.908 | 35.866 | 1.00 | 27.89 | C |
| ATOM | 1920 | CG  | GLU | A | 250 | 15.880 | 54.684 | 35.485 | 1.00 | 32.57 | C |
| ATOM | 1921 | CD  | GLU | A | 250 | 15.258 | 55.459 | 36.631 | 1.00 | 37.09 | C |
| ATOM | 1922 | OE1 | GLU | A | 250 | 15.809 | 55.491 | 37.753 | 1.00 | 42.28 | O |
| ATOM | 1923 | OE2 | GLU | A | 250 | 14.198 | 56.055 | 36.399 | 1.00 | 42.29 | O |
| ATOM | 1924 | N   | ARG | A | 251 | 19.042 | 51.399 | 35.490 | 1.00 | 25.57 | N |
| ATOM | 1925 | CA  | ARG | A | 251 | 20.224 | 50.657 | 35.900 | 1.00 | 24.72 | C |
| ATOM | 1926 | C   | ARG | A | 251 | 20.955 | 50.069 | 34.718 | 1.00 | 23.56 | C |
| ATOM | 1927 | O   | ARG | A | 251 | 22.150 | 49.919 | 34.769 | 1.00 | 22.92 | O |
| ATOM | 1928 | CB  | ARG | A | 251 | 19.845 | 49.520 | 36.845 | 1.00 | 25.64 | C |
| ATOM | 1929 | CG  | ARG | A | 251 | 19.435 | 49.957 | 38.255 | 1.00 | 26.79 | C |
| ATOM | 1930 | CD  | ARG | A | 251 | 18.858 | 48.815 | 39.123 | 1.00 | 30.01 | C |
| ATOM | 1931 | NE  | ARG | A | 251 | 19.900 | 47.875 | 39.540 | 1.00 | 31.06 | N |
| ATOM | 1932 | CZ  | ARG | A | 251 | 19.709 | 46.579 | 39.766 | 1.00 | 32.72 | C |
| ATOM | 1933 | NH1 | ARG | A | 251 | 18.508 | 46.029 | 39.628 | 1.00 | 33.10 | N |
| ATOM | 1934 | NH2 | ARG | A | 251 | 20.734 | 45.828 | 40.135 | 1.00 | 33.44 | N |
| ATOM | 1935 | N   | PHE | A | 252 | 20.234 | 49.725 | 33.652 | 1.00 | 22.66 | N |
| ATOM | 1936 | CA  | PHE | A | 252 | 20.826 | 49.019 | 32.532 | 1.00 | 21.99 | C |
| ATOM | 1937 | C   | PHE | A | 252 | 20.521 | 49.719 | 31.198 | 1.00 | 21.71 | C |
| ATOM | 1938 | O   | PHE | A | 252 | 19.900 | 49.160 | 30.289 | 1.00 | 21.32 | O |
| ATOM | 1939 | CB  | PHE | A | 252 | 20.261 | 47.610 | 32.519 | 1.00 | 22.03 | C |
| ATOM | 1940 | CG  | PHE | A | 252 | 20.292 | 46.915 | 33.868 | 1.00 | 21.75 | C |
| ATOM | 1941 | CD1 | PHE | A | 252 | 21.484 | 46.729 | 34.556 | 1.00 | 20.90 | C |
| ATOM | 1942 | CD2 | PHE | A | 252 | 19.124 | 46.402 | 34.423 | 1.00 | 21.94 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1943 | CE1 | PHE | A | 252 | 21.506 | 46.040 | 35.785 | 1.00 | 20.51 | C |
| ATOM | 1944 | CE2 | PHE | A | 252 | 19.136 | 45.730 | 35.662 | 1.00 | 21.77 | C |
| ATOM | 1945 | CZ  | PHE | A | 252 | 20.320 | 45.553 | 36.333 | 1.00 | 21.41 | C |
| ATOM | 1946 | N   | PRO | A | 253 | 20.989 | 50.944 | 31.071 | 1.00 | 20.88 | N |
| ATOM | 1947 | CA  | PRO | A | 253 | 20.615 | 51.754 | 29.909 | 1.00 | 20.51 | C |
| ATOM | 1948 | C   | PRO | A | 253 | 20.956 | 51.077 | 28.578 | 1.00 | 20.47 | C |
| ATOM | 1949 | O   | PRO | A | 253 | 20.153 | 51.159 | 27.656 | 1.00 | 20.01 | O |
| ATOM | 1950 | CB  | PRO | A | 253 | 21.371 | 53.077 | 30.130 | 1.00 | 20.00 | C |
| ATOM | 1951 | CG  | PRO | A | 253 | 22.538 | 52.697 | 31.136 | 1.00 | 20.46 | C |
| ATOM | 1952 | CD  | PRO | A | 253 | 21.921 | 51.641 | 31.994 | 1.00 | 20.89 | C |
| ATOM | 1953 | N   | ASN | A | 254 | 22.088 | 50.393 | 28.455 | 1.00 | 20.68 | N |
| ATOM | 1954 | CA  | ASN | A | 254 | 22.401 | 49.805 | 27.160 | 1.00 | 20.72 | C |
| ATOM | 1955 | C   | ASN | A | 254 | 21.537 | 48.601 | 26.790 | 1.00 | 20.29 | C |
| ATOM | 1956 | O   | ASN | A | 254 | 21.644 | 48.068 | 25.688 | 1.00 | 20.03 | O |
| ATOM | 1957 | CB  | ASN | A | 254 | 23.882 | 49.463 | 27.033 | 1.00 | 20.89 | C |
| ATOM | 1958 | CG  | ASN | A | 254 | 24.736 | 50.698 | 26.899 | 1.00 | 22.24 | C |
| ATOM | 1959 | OD1 | ASN | A | 254 | 25.532 | 50.999 | 27.785 | 1.00 | 24.48 | O |
| ATOM | 1960 | ND2 | ASN | A | 254 | 24.557 | 51.446 | 25.791 | 1.00 | 22.23 | N |
| ATOM | 1961 | N   | PHE | A | 255 | 20.678 | 48.160 | 27.690 | 1.00 | 20.01 | N |
| ATOM | 1962 | CA  | PHE | A | 255 | 19.781 | 47.086 | 27.305 | 1.00 | 20.02 | C |
| ATOM | 1963 | C   | PHE | A | 255 | 18.855 | 47.599 | 26.185 | 1.00 | 20.33 | C |
| ATOM | 1964 | O   | PHE | A | 255 | 18.224 | 46.818 | 25.472 | 1.00 | 19.82 | O |
| ATOM | 1965 | CB  | PHE | A | 255 | 18.970 | 46.552 | 28.484 | 1.00 | 19.63 | C |
| ATOM | 1966 | CG  | PHE | A | 255 | 18.239 | 45.318 | 28.145 | 1.00 | 18.96 | C |
| ATOM | 1967 | CD1 | PHE | A | 255 | 18.928 | 44.149 | 27.930 | 1.00 | 19.50 | C |
| ATOM | 1968 | CD2 | PHE | A | 255 | 16.889 | 45.335 | 27.942 | 1.00 | 17.83 | C |
| ATOM | 1969 | CE1 | PHE | A | 255 | 18.267 | 42.997 | 27.575 | 1.00 | 20.08 | C |
| ATOM | 1970 | CE2 | PHE | A | 255 | 16.230 | 44.206 | 27.561 | 1.00 | 17.77 | C |
| ATOM | 1971 | CZ  | PHE | A | 255 | 16.912 | 43.036 | 27.381 | 1.00 | 21.57 | C |
| ATOM | 1972 | N   | GLN | A | 256 | 18.788 | 48.919 | 26.035 | 1.00 | 20.15 | N |
| ATOM | 1973 | CA  | GLN | A | 256 | 17.973 | 49.533 | 24.986 | 1.00 | 20.63 | C |
| ATOM | 1974 | C   | GLN | A | 256 | 18.594 | 49.343 | 23.591 | 1.00 | 20.12 | C |
| ATOM | 1975 | O   | GLN | A | 256 | 17.955 | 49.612 | 22.592 | 1.00 | 19.87 | O |
| ATOM | 1976 | CB  | GLN | A | 256 | 17.787 | 51.036 | 25.272 | 1.00 | 20.67 | C |
| ATOM | 1977 | CG  | GLN | A | 256 | 16.744 | 51.306 | 26.362 | 1.00 | 22.56 | C |
| ATOM | 1978 | CD  | GLN | A | 256 | 16.747 | 52.732 | 26.888 | 1.00 | 22.75 | C |
| ATOM | 1979 | OE1 | GLN | A | 256 | 15.727 | 53.420 | 26.816 | 1.00 | 24.69 | O |
| ATOM | 1980 | NE2 | GLN | A | 256 | 17.873 | 53.172 | 27.419 | 1.00 | 23.90 | N |
| ATOM | 1981 | N   | ASN | A | 257 | 19.850 | 48.915 | 23.553 | 1.00 | 20.07 | N |
| ATOM | 1982 | CA  | ASN | A | 257 | 20.583 | 48.700 | 22.310 | 1.00 | 20.66 | C |
| ATOM | 1983 | C   | ASN | A | 257 | 20.778 | 47.233 | 21.963 | 1.00 | 21.21 | C |
| ATOM | 1984 | O   | ASN | A | 257 | 21.446 | 46.921 | 20.979 | 1.00 | 21.28 | O |
| ATOM | 1985 | CB  | ASN | A | 257 | 21.975 | 49.300 | 22.420 | 1.00 | 20.31 | C |
| ATOM | 1986 | CG  | ASN | A | 257 | 21.937 | 50.757 | 22.776 | 1.00 | 20.83 | C |
| ATOM | 1987 | OD1 | ASN | A | 257 | 22.395 | 51.141 | 23.850 | 1.00 | 20.15 | O |
| ATOM | 1988 | ND2 | ASN | A | 257 | 21.366 | 51.577 | 21.889 | 1.00 | 16.99 | N |
| ATOM | 1989 | N   | VAL | A | 258 | 20.218 | 46.333 | 22.758 | 1.00 | 21.91 | N |
| ATOM | 1990 | CA  | VAL | A | 258 | 20.440 | 44.908 | 22.532 | 1.00 | 23.55 | C |
| ATOM | 1991 | C   | VAL | A | 258 | 19.720 | 44.400 | 21.284 | 1.00 | 24.29 | C |
| ATOM | 1992 | O   | VAL | A | 258 | 18.600 | 44.845 | 20.947 | 1.00 | 24.28 | O |
| ATOM | 1993 | CB  | VAL | A | 258 | 20.026 | 44.110 | 23.772 | 1.00 | 24.18 | C |
| ATOM | 1994 | CG1 | VAL | A | 258 | 18.529 | 43.868 | 23.785 | 1.00 | 23.69 | C |
| ATOM | 1995 | CG2 | VAL | A | 258 | 20.761 | 42.851 | 23.826 | 1.00 | 28.07 | C |
| ATOM | 1996 | N   | VAL | A | 259 | 20.381 | 43.506 | 20.562 | 1.00 | 24.48 | N |
| ATOM | 1997 | CA  | VAL | A | 259 | 19.787 | 42.922 | 19.364 | 1.00 | 25.21 | C |
| ATOM | 1998 | C   | VAL | A | 259 | 20.104 | 41.427 | 19.331 | 1.00 | 25.19 | C |
| ATOM | 1999 | O   | VAL | A | 259 | 21.260 | 41.046 | 19.333 | 1.00 | 25.58 | O |
| ATOM | 2000 | CB  | VAL | A | 259 | 20.345 | 43.551 | 18.094 | 1.00 | 25.37 | C |
| ATOM | 2001 | CG1 | VAL | A | 259 | 19.726 | 42.893 | 16.882 | 1.00 | 27.15 | C |
| ATOM | 2002 | CG2 | VAL | A | 259 | 20.074 | 45.059 | 18.066 | 1.00 | 25.97 | C |
| ATOM | 2003 | N   | GLY | A | 260 | 19.068 | 40.603 | 19.308 | 1.00 | 25.20 | N |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2004 | CA  | GLY | A | 260 | 19.214 | 39.161 | 19.312 | 1.00 | 25.52 | C |
| ATOM | 2005 | C   | GLY | A | 260 | 19.108 | 38.433 | 17.961 | 1.00 | 25.26 | C |
| ATOM | 2006 | O   | GLY | A | 260 | 18.762 | 39.016 | 16.914 | 1.00 | 24.66 | O |
| ATOM | 2007 | N   | TYR | A | 261 | 19.484 | 37.160 | 18.015 | 1.00 | 24.49 | N |
| ATOM | 2008 | CA  | TYR | A | 261 | 19.379 | 36.217 | 16.925 | 1.00 | 25.05 | C |
| ATOM | 2009 | C   | TYR | A | 261 | 18.435 | 35.145 | 17.475 | 1.00 | 24.39 | C |
| ATOM | 2010 | O   | TYR | A | 261 | 18.671 | 34.620 | 18.552 | 1.00 | 23.82 | O |
| ATOM | 2011 | CB  | TYR | A | 261 | 20.730 | 35.574 | 16.627 | 1.00 | 25.82 | C |
| ATOM | 2012 | CG  | TYR | A | 261 | 21.748 | 36.476 | 15.965 | 1.00 | 28.98 | C |
| ATOM | 2013 | CD1 | TYR | A | 261 | 21.804 | 36.598 | 14.585 | 1.00 | 35.41 | C |
| ATOM | 2014 | CD2 | TYR | A | 261 | 22.649 | 37.194 | 16.712 | 1.00 | 29.78 | C |
| ATOM | 2015 | CE1 | TYR | A | 261 | 22.737 | 37.429 | 13.976 | 1.00 | 35.73 | C |
| ATOM | 2016 | CE2 | TYR | A | 261 | 23.592 | 37.994 | 16.126 | 1.00 | 32.54 | C |
| ATOM | 2017 | CZ  | TYR | A | 261 | 23.643 | 38.116 | 14.768 | 1.00 | 35.98 | C |
| ATOM | 2018 | OH  | TYR | A | 261 | 24.580 | 38.959 | 14.202 | 1.00 | 38.02 | O |
| ATOM | 2019 | N   | GLU | A | 262 | 17.353 | 34.823 | 16.790 | 1.00 | 24.04 | N |
| ATOM | 2020 | CA  | GLU | A | 262 | 16.432 | 33.860 | 17.387 | 1.00 | 23.96 | C |
| ATOM | 2021 | C   | GLU | A | 262 | 15.992 | 32.773 | 16.435 | 1.00 | 23.90 | C |
| ATOM | 2022 | O   | GLU | A | 262 | 16.116 | 32.890 | 15.213 | 1.00 | 23.56 | O |
| ATOM | 2023 | CB  | GLU | A | 262 | 15.224 | 34.553 | 18.020 | 1.00 | 23.70 | C |
| ATOM | 2024 | CG  | GLU | A | 262 | 14.029 | 34.782 | 17.127 | 1.00 | 24.33 | C |
| ATOM | 2025 | CD  | GLU | A | 262 | 12.829 | 35.382 | 17.870 | 1.00 | 26.49 | C |
| ATOM | 2026 | OE1 | GLU | A | 262 | 12.753 | 36.611 | 18.029 | 1.00 | 27.38 | O |
| ATOM | 2027 | OE2 | GLU | A | 262 | 11.946 | 34.631 | 18.306 | 1.00 | 28.26 | O |
| ATOM | 2028 | N   | THR | A | 263 | 15.485 | 31.713 | 17.034 | 1.00 | 23.68 | N |
| ATOM | 2029 | CA  | THR | A | 263 | 14.974 | 30.605 | 16.279 | 1.00 | 24.40 | C |
| ATOM | 2030 | C   | THR | A | 263 | 14.091 | 29.786 | 17.193 | 1.00 | 24.29 | C |
| ATOM | 2031 | O   | THR | A | 263 | 14.131 | 29.936 | 18.423 | 1.00 | 24.53 | O |
| ATOM | 2032 | CB  | THR | A | 263 | 16.148 | 29.762 | 15.751 | 1.00 | 24.52 | C |
| ATOM | 2033 | OG1 | THR | A | 263 | 15.684 | 28.839 | 14.762 | 1.00 | 24.43 | O |
| ATOM | 2034 | CG2 | THR | A | 263 | 16.737 | 28.876 | 16.854 | 1.00 | 24.33 | C |
| ATOM | 2035 | N   | VAL | A | 264 | 13.263 | 28.954 | 16.593 | 1.00 | 23.62 | N |
| ATOM | 2036 | CA  | VAL | A | 264 | 12.500 | 28.019 | 17.370 | 1.00 | 24.01 | C |
| ATOM | 2037 | C   | VAL | A | 264 | 12.936 | 26.627 | 16.935 | 1.00 | 24.53 | C |
| ATOM | 2038 | O   | VAL | A | 264 | 12.879 | 26.291 | 15.768 | 1.00 | 24.27 | O |
| ATOM | 2039 | CB  | VAL | A | 264 | 11.008 | 28.194 | 17.177 | 1.00 | 24.69 | C |
| ATOM | 2040 | CG1 | VAL | A | 264 | 10.256 | 26.958 | 17.712 | 1.00 | 23.69 | C |
| ATOM | 2041 | CG2 | VAL | A | 264 | 10.520 | 29.526 | 17.857 | 1.00 | 23.81 | C |
| ATOM | 2042 | N   | VAL | A | 265 | 13.450 | 25.844 | 17.872 | 1.00 | 24.91 | N |
| ATOM | 2043 | CA  | VAL | A | 265 | 13.833 | 24.484 | 17.540 | 1.00 | 24.93 | C |
| ATOM | 2044 | C   | VAL | A | 265 | 12.792 | 23.470 | 17.967 | 1.00 | 24.20 | C |
| ATOM | 2045 | O   | VAL | A | 265 | 12.167 | 23.617 | 19.018 | 1.00 | 24.01 | O |
| ATOM | 2046 | CB  | VAL | A | 265 | 15.196 | 24.072 | 18.173 | 1.00 | 25.05 | C |
| ATOM | 2047 | CG1 | VAL | A | 265 | 16.291 | 24.884 | 17.557 | 1.00 | 26.38 | C |
| ATOM | 2048 | CG2 | VAL | A | 265 | 15.190 | 24.164 | 19.702 | 1.00 | 23.59 | C |
| ATOM | 2049 | N   | GLY | A | 266 | 12.641 | 22.439 | 17.144 | 1.00 | 23.26 | N |
| ATOM | 2050 | CA  | GLY | A | 266 | 11.776 | 21.316 | 17.451 | 1.00 | 23.22 | C |
| ATOM | 2051 | C   | GLY | A | 266 | 12.467 | 19.961 | 17.359 | 1.00 | 22.26 | C |
| ATOM | 2052 | O   | GLY | A | 266 | 13.661 | 19.872 | 17.131 | 1.00 | 22.37 | O |
| ATOM | 2053 | N   | PRO | A | 267 | 11.712 | 18.884 | 17.524 | 1.00 | 21.90 | N |
| ATOM | 2054 | CA  | PRO | A | 267 | 12.305 | 17.544 | 17.479 | 1.00 | 21.60 | C |
| ATOM | 2055 | C   | PRO | A | 267 | 13.206 | 17.355 | 16.280 | 1.00 | 20.82 | C |
| ATOM | 2056 | O   | PRO | A | 267 | 12.768 | 17.588 | 15.169 | 1.00 | 20.29 | O |
| ATOM | 2057 | CB  | PRO | A | 267 | 11.086 | 16.622 | 17.364 | 1.00 | 21.36 | C |
| ATOM | 2058 | CG  | PRO | A | 267 | 10.023 | 17.330 | 18.028 | 1.00 | 23.23 | C |
| ATOM | 2059 | CD  | PRO | A | 267 | 10.254 | 18.831 | 17.753 | 1.00 | 21.99 | C |
| ATOM | 2060 | N   | GLY | A | 268 | 14.445 | 16.938 | 16.496 | 1.00 | 20.81 | N |
| ATOM | 2061 | CA  | GLY | A | 268 | 15.340 | 16.674 | 15.383 | 1.00 | 20.31 | C |
| ATOM | 2062 | C   | GLY | A | 268 | 16.296 | 17.806 | 15.111 | 1.00 | 20.37 | C |
| ATOM | 2063 | O   | GLY | A | 268 | 17.333 | 17.605 | 14.476 | 1.00 | 21.79 | O |
| ATOM | 2064 | N   | ASP | A | 269 | 15.975 | 19.002 | 15.582 | 1.00 | 19.89 | N |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2065 | CA  | ASP | A | 269 | 16.849 | 20.141 | 15.364 | 1.00 | 19.78 | C |
| ATOM | 2066 | C   | ASP | A | 269 | 17.991 | 20.162 | 16.395 | 1.00 | 19.63 | C |
| ATOM | 2067 | O   | ASP | A | 269 | 17.829 | 19.729 | 17.551 | 1.00 | 18.28 | O |
| ATOM | 2068 | CB  | ASP | A | 269 | 16.069 | 21.436 | 15.532 | 1.00 | 20.34 | C |
| ATOM | 2069 | CG  | ASP | A | 269 | 14.976 | 21.636 | 14.500 | 1.00 | 20.66 | C |
| ATOM | 2070 | OD1 | ASP | A | 269 | 14.977 | 21.015 | 13.419 | 1.00 | 22.15 | O |
| ATOM | 2071 | OD2 | ASP | A | 269 | 14.072 | 22.454 | 14.703 | 1.00 | 23.30 | O |
| ATOM | 2072 | N   | VAL | A | 270 | 19.129 | 20.681 | 15.953 | 1.00 | 19.76 | N |
| ATOM | 2073 | CA  | VAL | A | 270 | 20.304 | 20.879 | 16.782 | 1.00 | 20.24 | C |
| ATOM | 2074 | C   | VAL | A | 270 | 20.793 | 22.318 | 16.601 | 1.00 | 19.84 | C |
| ATOM | 2075 | O   | VAL | A | 270 | 21.052 | 22.754 | 15.487 | 1.00 | 19.90 | O |
| ATOM | 2076 | CB  | VAL | A | 270 | 21.421 | 19.942 | 16.377 | 1.00 | 20.08 | C |
| ATOM | 2077 | CG1 | VAL | A | 270 | 22.676 | 20.288 | 17.121 | 1.00 | 21.38 | C |
| ATOM | 2078 | CG2 | VAL | A | 270 | 21.017 | 18.521 | 16.671 | 1.00 | 21.15 | C |
| ATOM | 2079 | N   | LEU | A | 271 | 20.885 | 23.056 | 17.699 | 1.00 | 19.86 | N |
| ATOM | 2080 | CA  | LEU | A | 271 | 21.341 | 24.427 | 17.656 | 1.00 | 20.03 | C |
| ATOM | 2081 | C   | LEU | A | 271 | 22.757 | 24.465 | 18.202 | 1.00 | 20.23 | C |
| ATOM | 2082 | O   | LEU | A | 271 | 23.032 | 23.946 | 19.276 | 1.00 | 19.73 | O |
| ATOM | 2083 | CB  | LEU | A | 271 | 20.429 | 25.328 | 18.465 | 1.00 | 20.59 | C |
| ATOM | 2084 | CG  | LEU | A | 271 | 20.934 | 26.742 | 18.724 | 1.00 | 20.93 | C |
| ATOM | 2085 | CD1 | LEU | A | 271 | 21.011 | 27.562 | 17.431 | 1.00 | 20.35 | C |
| ATOM | 2086 | CD2 | LEU | A | 271 | 20.039 | 27.428 | 19.728 | 1.00 | 22.31 | C |
| ATOM | 2087 | N   | TYR | A | 272 | 23.669 | 25.024 | 17.416 | 1.00 | 20.58 | N |
| ATOM | 2088 | CA  | TYR | A | 272 | 25.010 | 25.229 | 17.883 | 1.00 | 20.58 | C |
| ATOM | 2089 | C   | TYR | A | 272 | 24.985 | 26.535 | 18.653 | 1.00 | 20.69 | C |
| ATOM | 2090 | O   | TYR | A | 272 | 24.692 | 27.576 | 18.089 | 1.00 | 21.54 | O |
| ATOM | 2091 | CB  | TYR | A | 272 | 26.004 | 25.312 | 16.728 | 1.00 | 20.30 | C |
| ATOM | 2092 | CG  | TYR | A | 272 | 27.381 | 25.776 | 17.158 | 1.00 | 21.24 | C |
| ATOM | 2093 | CD1 | TYR | A | 272 | 27.997 | 25.250 | 18.275 | 1.00 | 21.70 | C |
| ATOM | 2094 | CD2 | TYR | A | 272 | 28.039 | 26.788 | 16.472 | 1.00 | 22.21 | C |
| ATOM | 2095 | CE1 | TYR | A | 272 | 29.232 | 25.692 | 18.674 | 1.00 | 21.69 | C |
| ATOM | 2096 | CE2 | TYR | A | 272 | 29.275 | 27.215 | 16.857 | 1.00 | 22.99 | C |
| ATOM | 2097 | CZ  | TYR | A | 272 | 29.868 | 26.672 | 17.961 | 1.00 | 22.01 | C |
| ATOM | 2098 | OH  | TYR | A | 272 | 31.109 | 27.111 | 18.352 | 1.00 | 22.77 | O |
| ATOM | 2099 | N   | ILE | A | 273 | 25.216 | 26.454 | 19.951 | 1.00 | 21.22 | N |
| ATOM | 2100 | CA  | ILE | A | 273 | 25.362 | 27.629 | 20.805 | 1.00 | 21.49 | C |
| ATOM | 2101 | C   | ILE | A | 273 | 26.852 | 27.809 | 21.117 | 1.00 | 22.00 | C |
| ATOM | 2102 | O   | ILE | A | 273 | 27.413 | 27.112 | 21.962 | 1.00 | 22.55 | O |
| ATOM | 2103 | CB  | ILE | A | 273 | 24.607 | 27.471 | 22.073 | 1.00 | 21.14 | C |
| ATOM | 2104 | CG1 | ILE | A | 273 | 23.148 | 27.132 | 21.776 | 1.00 | 21.68 | C |
| ATOM | 2105 | CG2 | ILE | A | 273 | 24.661 | 28.791 | 22.854 | 1.00 | 21.75 | C |
| ATOM | 2106 | CD1 | ILE | A | 273 | 22.318 | 26.972 | 23.026 | 1.00 | 21.44 | C |
| ATOM | 2107 | N   | PRO | A | 274 | 27.493 | 28.723 | 20.413 | 1.00 | 21.86 | N |
| ATOM | 2108 | CA  | PRO | A | 274 | 28.929 | 28.916 | 20.557 | 1.00 | 22.49 | C |
| ATOM | 2109 | C   | PRO | A | 274 | 29.278 | 29.462 | 21.926 | 1.00 | 22.77 | C |
| ATOM | 2110 | O   | PRO | A | 274 | 28.510 | 30.231 | 22.521 | 1.00 | 21.72 | O |
| ATOM | 2111 | CB  | PRO | A | 274 | 29.305 | 29.908 | 19.429 | 1.00 | 23.00 | C |
| ATOM | 2112 | CG  | PRO | A | 274 | 28.022 | 30.225 | 18.658 | 1.00 | 23.03 | C |
| ATOM | 2113 | CD  | PRO | A | 274 | 26.889 | 29.582 | 19.398 | 1.00 | 22.21 | C |
| ATOM | 2114 | N   | MET | A | 275 | 30.441 | 29.028 | 22.404 | 1.00 | 22.72 | N |
| ATOM | 2115 | CA  | MET | A | 275 | 30.962 | 29.403 | 23.702 | 1.00 | 23.40 | C |
| ATOM | 2116 | C   | MET | A | 275 | 30.949 | 30.921 | 23.864 | 1.00 | 22.42 | C |
| ATOM | 2117 | O   | MET | A | 275 | 31.282 | 31.636 | 22.937 | 1.00 | 20.73 | O |
| ATOM | 2118 | CB  | MET | A | 275 | 32.373 | 28.856 | 23.826 | 1.00 | 23.99 | C |
| ATOM | 2119 | CG  | MET | A | 275 | 32.933 | 28.944 | 25.203 | 1.00 | 28.99 | C |
| ATOM | 2120 | SD  | MET | A | 275 | 34.517 | 28.083 | 25.337 | 1.00 | 35.05 | S |
| ATOM | 2121 | CE  | MET | A | 275 | 35.287 | 28.525 | 23.832 | 1.00 | 31.30 | C |
| ATOM | 2122 | N   | TYR | A | 276 | 30.509 | 31.388 | 25.030 | 1.00 | 22.30 | N |
| ATOM | 2123 | CA  | TYR | A | 276 | 30.419 | 32.831 | 25.349 | 1.00 | 23.06 | C |
| ATOM | 2124 | C   | TYR | A | 276 | 29.221 | 33.543 | 24.752 | 1.00 | 22.11 | C |
| ATOM | 2125 | O   | TYR | A | 276 | 29.012 | 34.705 | 25.041 | 1.00 | 21.84 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2126 | CB  | TYR | A | 276 | 31.673 | 33.594 | 24.934 | 1.00 | 23.42 | C |
| ATOM | 2127 | CG  | TYR | A | 276 | 32.857 | 33.283 | 25.796 | 1.00 | 28.51 | C |
| ATOM | 2128 | CD1 | TYR | A | 276 | 32.969 | 33.799 | 27.072 | 1.00 | 33.00 | C |
| ATOM | 2129 | CD2 | TYR | A | 276 | 33.876 | 32.460 | 25.321 | 1.00 | 34.41 | C |
| ATOM | 2130 | CE1 | TYR | A | 276 | 34.066 | 33.490 | 27.877 | 1.00 | 36.36 | C |
| ATOM | 2131 | CE2 | TYR | A | 276 | 34.968 | 32.151 | 26.102 | 1.00 | 36.45 | C |
| ATOM | 2132 | CZ  | TYR | A | 276 | 35.059 | 32.651 | 27.371 | 1.00 | 37.63 | C |
| ATOM | 2133 | OH  | TYR | A | 276 | 36.192 | 32.314 | 28.077 | 1.00 | 40.88 | O |
| ATOM | 2134 | N   | TRP | A | 277 | 28.455 | 32.878 | 23.906 | 1.00 | 20.75 | N |
| ATOM | 2135 | CA  | TRP | A | 277 | 27.272 | 33.528 | 23.360 | 1.00 | 20.85 | C |
| ATOM | 2136 | C   | TRP | A | 277 | 26.173 | 33.482 | 24.372 | 1.00 | 20.33 | C |
| ATOM | 2137 | O   | TRP | A | 277 | 25.907 | 32.431 | 24.949 | 1.00 | 20.72 | O |
| ATOM | 2138 | CB  | TRP | A | 277 | 26.791 | 32.874 | 22.068 | 1.00 | 20.13 | C |
| ATOM | 2139 | CG  | TRP | A | 277 | 27.552 | 33.323 | 20.879 | 1.00 | 19.28 | C |
| ATOM | 2140 | CD1 | TRP | A | 277 | 28.887 | 33.175 | 20.673 | 1.00 | 21.27 | C |
| ATOM | 2141 | CD2 | TRP | A | 277 | 27.042 | 33.995 | 19.730 | 1.00 | 20.60 | C |
| ATOM | 2142 | NE1 | TRP | A | 277 | 29.246 | 33.721 | 19.467 | 1.00 | 21.05 | N |
| ATOM | 2143 | CE2 | TRP | A | 277 | 28.128 | 34.232 | 18.864 | 1.00 | 21.04 | C |
| ATOM | 2144 | CE3 | TRP | A | 277 | 25.780 | 34.456 | 19.352 | 1.00 | 21.08 | C |
| ATOM | 2145 | CZ2 | TRP | A | 277 | 27.989 | 34.893 | 17.643 | 1.00 | 20.38 | C |
| ATOM | 2146 | CZ3 | TRP | A | 277 | 25.641 | 35.110 | 18.122 | 1.00 | 20.48 | C |
| ATOM | 2147 | CH2 | TRP | A | 277 | 26.736 | 35.306 | 17.288 | 1.00 | 21.03 | C |
| ATOM | 2148 | N   | TRP | A | 278 | 25.572 | 34.632 | 24.629 | 1.00 | 19.39 | N |
| ATOM | 2149 | CA  | TRP | A | 278 | 24.430 | 34.711 | 25.521 | 1.00 | 19.80 | C |
| ATOM | 2150 | C   | TRP | A | 278 | 23.243 | 33.927 | 24.927 | 1.00 | 20.18 | C |
| ATOM | 2151 | O   | TRP | A | 278 | 23.019 | 33.939 | 23.732 | 1.00 | 21.04 | O |
| ATOM | 2152 | CB  | TRP | A | 278 | 23.989 | 36.168 | 25.646 | 1.00 | 20.39 | C |
| ATOM | 2153 | CG  | TRP | A | 278 | 24.979 | 37.031 | 26.300 | 1.00 | 21.20 | C |
| ATOM | 2154 | CD1 | TRP | A | 278 | 26.022 | 37.672 | 25.720 | 1.00 | 21.06 | C |
| ATOM | 2155 | CD2 | TRP | A | 278 | 25.056 | 37.301 | 27.691 | 1.00 | 20.38 | C |
| ATOM | 2156 | NE1 | TRP | A | 278 | 26.725 | 38.369 | 26.668 | 1.00 | 22.44 | N |
| ATOM | 2157 | CE2 | TRP | A | 278 | 26.139 | 38.155 | 27.891 | 1.00 | 21.86 | C |
| ATOM | 2158 | CE3 | TRP | A | 278 | 24.282 | 36.937 | 28.789 | 1.00 | 21.09 | C |
| ATOM | 2159 | CZ2 | TRP | A | 278 | 26.480 | 38.640 | 29.147 | 1.00 | 21.13 | C |
| ATOM | 2160 | CZ3 | TRP | A | 278 | 24.623 | 37.412 | 30.019 | 1.00 | 23.38 | C |
| ATOM | 2161 | CH2 | TRP | A | 278 | 25.704 | 38.258 | 30.194 | 1.00 | 21.06 | C |
| ATOM | 2162 | N   | HIS | A | 279 | 22.465 | 33.278 | 25.761 | 1.00 | 20.76 | N |
| ATOM | 2163 | CA  | HIS | A | 279 | 21.262 | 32.646 | 25.294 | 1.00 | 21.56 | C |
| ATOM | 2164 | C   | HIS | A | 279 | 20.198 | 32.659 | 26.361 | 1.00 | 21.24 | C |
| ATOM | 2165 | O   | HIS | A | 279 | 20.475 | 32.456 | 27.540 | 1.00 | 21.63 | O |
| ATOM | 2166 | CB  | HIS | A | 279 | 21.501 | 31.203 | 24.819 | 1.00 | 21.83 | C |
| ATOM | 2167 | CG  | HIS | A | 279 | 22.342 | 30.379 | 25.738 | 1.00 | 23.50 | C |
| ATOM | 2168 | ND1 | HIS | A | 279 | 23.713 | 30.494 | 25.785 | 1.00 | 24.98 | N |
| ATOM | 2169 | CD2 | HIS | A | 279 | 22.017 | 29.385 | 26.602 | 1.00 | 26.21 | C |
| ATOM | 2170 | CE1 | HIS | A | 279 | 24.200 | 29.599 | 26.628 | 1.00 | 26.46 | C |
| ATOM | 2171 | NE2 | HIS | A | 279 | 23.192 | 28.927 | 27.158 | 1.00 | 25.14 | N |
| ATOM | 2172 | N   | HIS | A | 280 | 18.994 | 32.900 | 25.874 | 1.00 | 21.71 | N |
| ATOM | 2173 | CA  | HIS | A | 280 | 17.736 | 32.956 | 26.602 | 1.00 | 21.78 | C |
| ATOM | 2174 | C   | HIS | A | 280 | 16.890 | 31.860 | 25.951 | 1.00 | 21.70 | C |
| ATOM | 2175 | O   | HIS | A | 280 | 16.722 | 31.846 | 24.736 | 1.00 | 21.40 | O |
| ATOM | 2176 | CB  | HIS | A | 280 | 17.104 | 34.322 | 26.374 | 1.00 | 21.20 | C |
| ATOM | 2177 | CG  | HIS | A | 280 | 15.642 | 34.367 | 26.626 | 1.00 | 21.64 | C |
| ATOM | 2178 | ND1 | HIS | A | 280 | 15.100 | 35.028 | 27.705 | 1.00 | 22.67 | N |
| ATOM | 2179 | CD2 | HIS | A | 280 | 14.600 | 33.826 | 25.951 | 1.00 | 23.33 | C |
| ATOM | 2180 | CE1 | HIS | A | 280 | 13.786 | 34.891 | 27.684 | 1.00 | 23.20 | C |
| ATOM | 2181 | NE2 | HIS | A | 280 | 13.457 | 34.158 | 26.635 | 1.00 | 23.30 | N |
| ATOM | 2182 | N   | ILE | A | 281 | 16.368 | 30.934 | 26.733 | 1.00 | 22.98 | N |
| ATOM | 2183 | CA  | ILE | A | 281 | 15.658 | 29.779 | 26.158 | 1.00 | 23.36 | C |
| ATOM | 2184 | C   | ILE | A | 281 | 14.313 | 29.606 | 26.800 | 1.00 | 23.58 | C |
| ATOM | 2185 | O   | ILE | A | 281 | 14.209 | 29.592 | 28.014 | 1.00 | 23.63 | O |
| ATOM | 2186 | CB  | ILE | A | 281 | 16.512 | 28.525 | 26.301 | 1.00 | 23.87 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2187 | CG1 | ILE | A | 281 | 17.771 | 28.675 | 25.435 | 1.00 | 25.77 | C |
| ATOM | 2188 | CG2 | ILE | A | 281 | 15.748 | 27.261 | 25.863 | 1.00 | 23.54 | C |
| ATOM | 2189 | CD1 | ILE | A | 281 | 18.752 | 27.659 | 25.690 | 1.00 | 29.36 | C |
| ATOM | 2190 | N   | GLU | A | 282 | 13.268 | 29.510 | 25.982 | 1.00 | 23.92 | N |
| ATOM | 2191 | CA  | GLU | A | 282 | 11.923 | 29.337 | 26.525 | 1.00 | 24.26 | C |
| ATOM | 2192 | C   | GLU | A | 282 | 11.113 | 28.234 | 25.834 | 1.00 | 23.82 | C |
| ATOM | 2193 | O   | GLU | A | 282 | 11.115 | 28.107 | 24.606 | 1.00 | 24.00 | O |
| ATOM | 2194 | CB  | GLU | A | 282 | 11.166 | 30.681 | 26.490 | 1.00 | 24.35 | C |
| ATOM | 2195 | CG  | GLU | A | 282 | 10.887 | 31.249 | 25.112 | 1.00 | 25.59 | C |
| ATOM | 2196 | CD  | GLU | A | 282 | 10.320 | 32.668 | 25.168 | 1.00 | 25.45 | C |
| ATOM | 2197 | OE1 | GLU | A | 282 | 10.861 | 33.494 | 25.929 | 1.00 | 26.04 | O |
| ATOM | 2198 | OE2 | GLU | A | 282 | 9.332  | 32.954 | 24.451 | 1.00 | 25.08 | O |
| ATOM | 2199 | N   | SER | A | 283 | 10.460 | 27.419 | 26.648 | 1.00 | 23.28 | N |
| ATOM | 2200 | CA  | SER | A | 283 | 9.573  | 26.373 | 26.166 | 1.00 | 23.66 | C |
| ATOM | 2201 | C   | SER | A | 283 | 8.257  | 27.054 | 25.787 | 1.00 | 23.86 | C |
| ATOM | 2202 | O   | SER | A | 283 | 7.678  | 27.780 | 26.593 | 1.00 | 23.20 | O |
| ATOM | 2203 | CB  | SER | A | 283 | 9.341  | 25.321 | 27.247 | 1.00 | 23.36 | C |
| ATOM | 2204 | OG  | SER | A | 283 | 10.473 | 24.497 | 27.401 | 1.00 | 23.30 | O |
| ATOM | 2205 | N   | LEU | A | 284 | 7.792  | 26.837 | 24.564 | 1.00 | 24.56 | N |
| ATOM | 2206 | CA  | LEU | A | 284 | 6.626  | 27.583 | 24.084 | 1.00 | 25.62 | C |
| ATOM | 2207 | C   | LEU | A | 284 | 5.401  | 27.487 | 25.004 | 1.00 | 25.52 | C |
| ATOM | 2208 | O   | LEU | A | 284 | 5.114  | 26.431 | 25.589 | 1.00 | 24.71 | O |
| ATOM | 2209 | CB  | LEU | A | 284 | 6.237  | 27.157 | 22.680 | 1.00 | 25.64 | C |
| ATOM | 2210 | CG  | LEU | A | 284 | 7.274  | 27.308 | 21.576 | 1.00 | 27.12 | C |
| ATOM | 2211 | CD1 | LEU | A | 284 | 6.591  | 27.546 | 20.242 | 1.00 | 28.93 | C |
| ATOM | 2212 | CD2 | LEU | A | 284 | 8.248  | 28.364 | 21.851 | 1.00 | 27.08 | C |
| ATOM | 2213 | N   | LEU | A | 285 | 4.713  | 28.615 | 25.144 | 1.00 | 25.85 | N |
| ATOM | 2214 | CA  | LEU | A | 285 | 3.490  | 28.676 | 25.942 | 1.00 | 26.84 | C |
| ATOM | 2215 | C   | LEU | A | 285 | 2.507  | 27.691 | 25.345 | 1.00 | 27.10 | C |
| ATOM | 2216 | O   | LEU | A | 285 | 2.424  | 27.565 | 24.139 | 1.00 | 27.10 | O |
| ATOM | 2217 | CB  | LEU | A | 285 | 2.875  | 30.071 | 25.906 | 1.00 | 26.48 | C |
| ATOM | 2218 | CG  | LEU | A | 285 | 3.709  | 31.225 | 26.438 | 1.00 | 27.70 | C |
| ATOM | 2219 | CD1 | LEU | A | 285 | 3.075  | 32.554 | 26.026 | 1.00 | 28.22 | C |
| ATOM | 2220 | CD2 | LEU | A | 285 | 3.845  | 31.125 | 27.928 | 1.00 | 28.39 | C |
| ATOM | 2221 | N   | ASN | A | 286 | 1.779  | 26.987 | 26.196 | 1.00 | 27.81 | N |
| ATOM | 2222 | CA  | ASN | A | 286 | 0.790  | 26.007 | 25.753 | 1.00 | 28.27 | C |
| ATOM | 2223 | C   | ASN | A | 286 | 1.313  | 24.977 | 24.744 | 1.00 | 27.42 | C |
| ATOM | 2224 | O   | ASN | A | 286 | 0.555  | 24.481 | 23.922 | 1.00 | 26.50 | O |
| ATOM | 2225 | CB  | ASN | A | 286 | -0.417 | 26.741 | 25.160 | 1.00 | 29.08 | C |
| ATOM | 2226 | CG  | ASN | A | 286 | -0.931 | 27.846 | 26.078 | 1.00 | 32.15 | C |
| ATOM | 2227 | OD1 | ASN | A | 286 | -1.484 | 27.577 | 27.154 | 1.00 | 34.93 | O |
| ATOM | 2228 | ND2 | ASN | A | 286 | -0.725 | 29.099 | 25.670 | 1.00 | 35.91 | N |
| ATOM | 2229 | N   | GLY | A | 287 | 2.608  | 24.672 | 24.799 | 1.00 | 26.54 | N |
| ATOM | 2230 | CA  | GLY | A | 287 | 3.201  | 23.727 | 23.879 | 1.00 | 25.64 | C |
| ATOM | 2231 | C   | GLY | A | 287 | 3.474  | 22.371 | 24.497 | 1.00 | 25.01 | C |
| ATOM | 2232 | O   | GLY | A | 287 | 4.031  | 21.502 | 23.829 | 1.00 | 24.77 | O |
| ATOM | 2233 | N   | GLY | A | 288 | 3.110  | 22.187 | 25.766 | 1.00 | 24.43 | N |
| ATOM | 2234 | CA  | GLY | A | 288 | 3.357  | 20.922 | 26.455 | 1.00 | 23.99 | C |
| ATOM | 2235 | C   | GLY | A | 288 | 4.804  | 20.844 | 26.935 | 1.00 | 24.11 | C |
| ATOM | 2236 | O   | GLY | A | 288 | 5.546  | 21.810 | 26.786 | 1.00 | 22.82 | O |
| ATOM | 2237 | N   | ILE | A | 289 | 5.211  | 19.695 | 27.472 | 1.00 | 23.99 | N |
| ATOM | 2238 | CA  | ILE | A | 289 | 6.550  | 19.522 | 28.000 | 1.00 | 24.69 | C |
| ATOM | 2239 | C   | ILE | A | 289 | 7.605  | 19.496 | 26.908 | 1.00 | 24.25 | C |
| ATOM | 2240 | O   | ILE | A | 289 | 7.350  | 19.092 | 25.774 | 1.00 | 25.20 | O |
| ATOM | 2241 | CB  | ILE | A | 289 | 6.691  | 18.234 | 28.836 | 1.00 | 25.39 | C |
| ATOM | 2242 | CG1 | ILE | A | 289 | 6.702  | 17.006 | 27.941 | 1.00 | 27.43 | C |
| ATOM | 2243 | CG2 | ILE | A | 289 | 5.613  | 18.151 | 29.921 | 1.00 | 26.30 | C |
| ATOM | 2244 | CD1 | ILE | A | 289 | 7.255  | 15.752 | 28.650 | 1.00 | 30.57 | C |
| ATOM | 2245 | N   | THR | A | 290 | 8.808  | 19.912 | 27.267 | 1.00 | 23.28 | N |
| ATOM | 2246 | CA  | THR | A | 290 | 9.908  | 19.908 | 26.334 | 1.00 | 22.12 | C |
| ATOM | 2247 | C   | THR | A | 290 | 11.008 | 18.984 | 26.824 | 1.00 | 21.52 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2248 | O   | THR | A | 290 | 11.193 | 18.789 | 28.029 | 1.00 | 20.85 | O |
| ATOM | 2249 | CB  | THR | A | 290 | 10.473 | 21.318 | 26.168 | 1.00 | 22.19 | C |
| ATOM | 2250 | OG1 | THR | A | 290 | 10.758 | 21.885 | 27.444 | 1.00 | 21.69 | O |
| ATOM | 2251 | CG2 | THR | A | 290 | 9.436  | 22.268 | 25.557 | 1.00 | 23.05 | C |
| ATOM | 2252 | N   | ILE | A | 291 | 11.746 | 18.421 | 25.880 | 1.00 | 20.44 | N |
| ATOM | 2253 | CA  | ILE | A | 291 | 12.880 | 17.616 | 26.234 | 1.00 | 21.24 | C |
| ATOM | 2254 | C   | ILE | A | 291 | 14.033 | 17.981 | 25.347 | 1.00 | 20.47 | C |
| ATOM | 2255 | O   | ILE | A | 291 | 13.869 | 18.064 | 24.137 | 1.00 | 21.04 | O |
| ATOM | 2256 | CB  | ILE | A | 291 | 12.559 | 16.118 | 26.078 | 1.00 | 21.40 | C |
| ATOM | 2257 | CG1 | ILE | A | 291 | 11.405 | 15.724 | 27.004 | 1.00 | 22.31 | C |
| ATOM | 2258 | CG2 | ILE | A | 291 | 13.798 | 15.310 | 26.383 | 1.00 | 22.63 | C |
| ATOM | 2259 | CD1 | ILE | A | 291 | 10.969 | 14.262 | 26.867 | 1.00 | 23.92 | C |
| ATOM | 2260 | N   | THR | A | 292 | 15.194 | 18.188 | 25.953 | 1.00 | 20.24 | N |
| ATOM | 2261 | CA  | THR | A | 292 | 16.395 | 18.517 | 25.236 | 1.00 | 20.13 | C |
| ATOM | 2262 | C   | THR | A | 292 | 17.560 | 17.794 | 25.831 | 1.00 | 20.29 | C |
| ATOM | 2263 | O   | THR | A | 292 | 17.605 | 17.557 | 27.021 | 1.00 | 20.94 | O |
| ATOM | 2264 | CB  | THR | A | 292 | 16.688 | 20.044 | 25.365 | 1.00 | 20.34 | C |
| ATOM | 2265 | OG1 | THR | A | 292 | 15.524 | 20.799 | 25.022 | 1.00 | 19.08 | O |
| ATOM | 2266 | CG2 | THR | A | 292 | 17.730 | 20.487 | 24.355 | 1.00 | 20.32 | C |
| ATOM | 2267 | N   | VAL | A | 293 | 18.530 | 17.454 | 25.003 | 1.00 | 20.52 | N |
| ATOM | 2268 | CA  | VAL | A | 293 | 19.784 | 16.939 | 25.516 | 1.00 | 20.48 | C |
| ATOM | 2269 | C   | VAL | A | 293 | 20.892 | 17.803 | 24.918 | 1.00 | 20.80 | C |
| ATOM | 2270 | O   | VAL | A | 293 | 20.936 | 17.954 | 23.709 | 1.00 | 19.58 | O |
| ATOM | 2271 | CB  | VAL | A | 293 | 19.995 | 15.483 | 25.129 | 1.00 | 20.78 | C |
| ATOM | 2272 | CG1 | VAL | A | 293 | 21.436 | 15.068 | 25.385 | 1.00 | 20.33 | C |
| ATOM | 2273 | CG2 | VAL | A | 293 | 19.047 | 14.597 | 25.919 | 1.00 | 20.95 | C |
| ATOM | 2274 | N   | ASN | A | 294 | 21.749 | 18.412 | 25.752 | 1.00 | 21.34 | N |
| ATOM | 2275 | CA  | ASN | A | 294 | 22.855 | 19.192 | 25.205 | 1.00 | 22.04 | C |
| ATOM | 2276 | C   | ASN | A | 294 | 24.144 | 18.362 | 25.204 | 1.00 | 22.29 | C |
| ATOM | 2277 | O   | ASN | A | 294 | 24.182 | 17.241 | 25.720 | 1.00 | 23.22 | O |
| ATOM | 2278 | CB  | ASN | A | 294 | 23.012 | 20.581 | 25.883 | 1.00 | 22.35 | C |
| ATOM | 2279 | CG  | ASN | A | 294 | 23.703 | 20.520 | 27.259 | 1.00 | 23.08 | C |
| ATOM | 2280 | OD1 | ASN | A | 294 | 24.240 | 19.493 | 27.628 | 1.00 | 22.91 | O |
| ATOM | 2281 | ND2 | ASN | A | 294 | 23.657 | 21.640 | 28.027 | 1.00 | 21.75 | N |
| ATOM | 2282 | N   | PHE | A | 295 | 25.168 | 18.903 | 24.565 | 1.00 | 22.27 | N |
| ATOM | 2283 | CA  | PHE | A | 295 | 26.467 | 18.269 | 24.452 | 1.00 | 22.31 | C |
| ATOM | 2284 | C   | PHE | A | 295 | 27.444 | 19.408 | 24.704 | 1.00 | 22.66 | C |
| ATOM | 2285 | O   | PHE | A | 295 | 27.602 | 20.299 | 23.865 | 1.00 | 23.12 | O |
| ATOM | 2286 | CB  | PHE | A | 295 | 26.709 | 17.748 | 23.040 | 1.00 | 22.32 | C |
| ATOM | 2287 | CG  | PHE | A | 295 | 25.871 | 16.568 | 22.653 | 1.00 | 22.18 | C |
| ATOM | 2288 | CD1 | PHE | A | 295 | 24.494 | 16.689 | 22.477 | 1.00 | 22.38 | C |
| ATOM | 2289 | CD2 | PHE | A | 295 | 26.465 | 15.336 | 22.441 | 1.00 | 21.44 | C |
| ATOM | 2290 | CE1 | PHE | A | 295 | 23.757 | 15.604 | 22.111 | 1.00 | 24.06 | C |
| ATOM | 2291 | CE2 | PHE | A | 295 | 25.718 | 14.248 | 22.064 | 1.00 | 19.77 | C |
| ATOM | 2292 | CZ  | PHE | A | 295 | 24.380 | 14.366 | 21.911 | 1.00 | 21.39 | C |
| ATOM | 2293 | N   | TRP | A | 296 | 28.062 | 19.403 | 25.869 | 1.00 | 22.66 | N |
| ATOM | 2294 | CA  | TRP | A | 296 | 28.998 | 20.450 | 26.256 | 1.00 | 23.09 | C |
| ATOM | 2295 | C   | TRP | A | 296 | 30.454 | 19.991 | 26.081 | 1.00 | 23.22 | C |
| ATOM | 2296 | O   | TRP | A | 296 | 30.865 | 18.932 | 26.595 | 1.00 | 22.78 | O |
| ATOM | 2297 | CB  | TRP | A | 296 | 28.734 | 20.834 | 27.707 | 1.00 | 22.89 | C |
| ATOM | 2298 | CG  | TRP | A | 296 | 27.830 | 22.013 | 27.906 | 1.00 | 23.61 | C |
| ATOM | 2299 | CD1 | TRP | A | 296 | 27.783 | 23.129 | 27.149 | 1.00 | 25.47 | C |
| ATOM | 2300 | CD2 | TRP | A | 296 | 26.894 | 22.219 | 28.975 | 1.00 | 24.55 | C |
| ATOM | 2301 | NE1 | TRP | A | 296 | 26.874 | 24.018 | 27.667 | 1.00 | 25.25 | N |
| ATOM | 2302 | CE2 | TRP | A | 296 | 26.308 | 23.478 | 28.783 | 1.00 | 24.33 | C |
| ATOM | 2303 | CE3 | TRP | A | 296 | 26.464 | 21.444 | 30.061 | 1.00 | 27.49 | C |
| ATOM | 2304 | CZ2 | TRP | A | 296 | 25.335 | 23.994 | 29.631 | 1.00 | 25.91 | C |
| ATOM | 2305 | CZ3 | TRP | A | 296 | 25.474 | 21.952 | 30.899 | 1.00 | 27.19 | C |
| ATOM | 2306 | CH2 | TRP | A | 296 | 24.935 | 23.224 | 30.682 | 1.00 | 26.96 | C |
| ATOM | 2307 | N   | TYR | A | 297 | 31.216 | 20.783 | 25.337 | 1.00 | 23.29 | N |
| ATOM | 2308 | CA  | TYR | A | 297 | 32.627 | 20.510 | 25.100 | 1.00 | 23.80 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2309 | C   | TYR | A | 297 | 33.506 | 21.660 | 25.554 | 1.00 | 24.51 | C |
| ATOM | 2310 | O   | TYR | A | 297 | 33.188 | 22.825 | 25.323 | 1.00 | 23.73 | O |
| ATOM | 2311 | CB  | TYR | A | 297 | 32.882 | 20.332 | 23.610 | 1.00 | 23.38 | C |
| ATOM | 2312 | CG  | TYR | A | 297 | 32.284 | 19.092 | 23.021 | 1.00 | 23.42 | C |
| ATOM | 2313 | CD1 | TYR | A | 297 | 30.940 | 19.053 | 22.641 | 1.00 | 23.90 | C |
| ATOM | 2314 | CD2 | TYR | A | 297 | 33.056 | 17.971 | 22.808 | 1.00 | 21.43 | C |
| ATOM | 2315 | CE1 | TYR | A | 297 | 30.394 | 17.920 | 22.089 | 1.00 | 23.32 | C |
| ATOM | 2316 | CE2 | TYR | A | 297 | 32.515 | 16.826 | 22.250 | 1.00 | 22.05 | C |
| ATOM | 2317 | CZ  | TYR | A | 297 | 31.186 | 16.806 | 21.905 | 1.00 | 21.88 | C |
| ATOM | 2318 | OH  | TYR | A | 297 | 30.644 | 15.669 | 21.365 | 1.00 | 21.30 | O |
| ATOM | 2319 | N   | LYS | A | 298 | 34.637 | 21.334 | 26.160 | 1.00 | 25.35 | N |
| ATOM | 2320 | CA  | LYS | A | 298 | 35.589 | 22.362 | 26.536 | 1.00 | 26.48 | C |
| ATOM | 2321 | C   | LYS | A | 298 | 36.070 | 23.017 | 25.268 | 1.00 | 26.23 | C |
| ATOM | 2322 | O   | LYS | A | 298 | 36.224 | 22.364 | 24.249 | 1.00 | 24.85 | O |
| ATOM | 2323 | CB  | LYS | A | 298 | 36.783 | 21.771 | 27.308 | 1.00 | 27.15 | C |
| ATOM | 2324 | CG  | LYS | A | 298 | 36.474 | 21.471 | 28.777 | 1.00 | 30.00 | C |
| ATOM | 2325 | CD  | LYS | A | 298 | 37.666 | 20.901 | 29.550 | 1.00 | 33.20 | C |
| ATOM | 2326 | CE  | LYS | A | 298 | 37.232 | 20.493 | 30.969 | 1.00 | 36.09 | C |
| ATOM | 2327 | NZ  | LYS | A | 298 | 38.299 | 19.766 | 31.764 | 1.00 | 39.03 | N |
| ATOM | 2328 | N   | GLY | A | 299 | 36.321 | 24.313 | 25.329 | 1.00 | 27.13 | N |
| ATOM | 2329 | CA  | GLY | A | 299 | 36.798 | 25.014 | 24.159 | 1.00 | 28.27 | C |
| ATOM | 2330 | C   | GLY | A | 299 | 38.229 | 24.649 | 23.837 | 1.00 | 29.23 | C |
| ATOM | 2331 | O   | GLY | A | 299 | 38.892 | 24.005 | 24.613 | 1.00 | 28.19 | O |
| ATOM | 2332 | N   | ALA | A | 300 | 38.674 | 25.046 | 22.660 | 1.00 | 31.78 | N |
| ATOM | 2333 | CA  | ALA | A | 300 | 40.046 | 24.852 | 22.233 | 1.00 | 34.32 | C |
| ATOM | 2334 | C   | ALA | A | 300 | 40.992 | 25.610 | 23.155 | 1.00 | 36.37 | C |
| ATOM | 2335 | O   | ALA | A | 300 | 40.573 | 26.430 | 23.956 | 1.00 | 35.96 | O |
| ATOM | 2336 | CB  | ALA | A | 300 | 40.210 | 25.355 | 20.806 | 1.00 | 34.38 | C |
| ATOM | 2337 | N   | PRO | A | 301 | 42.280 | 25.349 | 23.025 | 1.00 | 39.70 | N |
| ATOM | 2338 | CA  | PRO | A | 301 | 43.278 | 26.051 | 23.845 | 1.00 | 41.64 | C |
| ATOM | 2339 | C   | PRO | A | 301 | 43.465 | 27.482 | 23.386 | 1.00 | 43.35 | C |
| ATOM | 2340 | O   | PRO | A | 301 | 43.220 | 27.803 | 22.228 | 1.00 | 43.86 | O |
| ATOM | 2341 | CB  | PRO | A | 301 | 44.566 | 25.275 | 23.572 | 1.00 | 41.46 | C |
| ATOM | 2342 | CG  | PRO | A | 301 | 44.382 | 24.736 | 22.199 | 1.00 | 41.25 | C |
| ATOM | 2343 | CD  | PRO | A | 301 | 42.906 | 24.416 | 22.068 | 1.00 | 40.04 | C |
| ATOM | 2344 | N   | THR | A | 302 | 43.900 | 28.328 | 24.300 | 1.00 | 45.97 | N |
| ATOM | 2345 | CA  | THR | A | 302 | 44.214 | 29.715 | 24.001 | 1.00 | 47.77 | C |
| ATOM | 2346 | C   | THR | A | 302 | 45.593 | 29.713 | 23.362 | 1.00 | 48.92 | C |
| ATOM | 2347 | O   | THR | A | 302 | 46.532 | 29.251 | 24.006 | 1.00 | 49.23 | O |
| ATOM | 2348 | CB  | THR | A | 302 | 44.282 | 30.469 | 25.322 | 1.00 | 48.10 | C |
| ATOM | 2349 | OG1 | THR | A | 302 | 43.006 | 30.416 | 25.976 | 1.00 | 49.37 | O |
| ATOM | 2350 | CG2 | THR | A | 302 | 44.520 | 31.924 | 25.100 | 1.00 | 48.91 | C |
| ATOM | 2351 | N   | PRO | A | 303 | 45.761 | 30.248 | 22.148 | 1.00 | 50.22 | N |
| ATOM | 2352 | CA  | PRO | A | 303 | 47.064 | 30.150 | 21.474 | 1.00 | 50.62 | C |
| ATOM | 2353 | C   | PRO | A | 303 | 48.191 | 30.728 | 22.316 | 1.00 | 50.64 | C |
| ATOM | 2354 | O   | PRO | A | 303 | 47.883 | 31.390 | 23.307 | 1.00 | 50.98 | O |
| ATOM | 2355 | CB  | PRO | A | 303 | 46.877 | 30.986 | 20.202 | 1.00 | 50.93 | C |
| ATOM | 2356 | CG  | PRO | A | 303 | 45.407 | 30.999 | 19.968 | 1.00 | 50.70 | C |
| ATOM | 2357 | CD  | PRO | A | 303 | 44.814 | 31.064 | 21.360 | 1.00 | 50.45 | C |
| ATOM | 2358 | N   | GLU | A | 307 | 46.978 | 37.074 | 18.830 | 1.00 | 53.59 | N |
| ATOM | 2359 | CA  | GLU | A | 307 | 46.946 | 38.016 | 17.714 | 1.00 | 53.82 | C |
| ATOM | 2360 | C   | GLU | A | 307 | 45.902 | 39.090 | 17.922 | 1.00 | 52.97 | C |
| ATOM | 2361 | O   | GLU | A | 307 | 44.792 | 38.810 | 18.358 | 1.00 | 53.64 | O |
| ATOM | 2362 | CB  | GLU | A | 307 | 46.672 | 37.308 | 16.371 | 1.00 | 54.37 | C |
| ATOM | 2363 | CG  | GLU | A | 307 | 46.875 | 38.231 | 15.159 | 1.00 | 56.16 | C |
| ATOM | 2364 | CD  | GLU | A | 307 | 46.966 | 37.504 | 13.822 | 1.00 | 57.96 | C |
| ATOM | 2365 | OE1 | GLU | A | 307 | 46.621 | 36.303 | 13.738 | 1.00 | 59.31 | O |
| ATOM | 2366 | OE2 | GLU | A | 307 | 47.388 | 38.150 | 12.839 | 1.00 | 59.69 | O |
| ATOM | 2367 | N   | TYR | A | 308 | 46.267 | 40.324 | 17.610 | 1.00 | 51.95 | N |
| ATOM | 2368 | CA  | TYR | A | 308 | 45.343 | 41.436 | 17.702 | 1.00 | 51.19 | C |
| ATOM | 2369 | C   | TYR | A | 308 | 44.693 | 41.603 | 16.337 | 1.00 | 50.27 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2370 | O   | TYR | A | 308 | 45.246 | 41.146 | 15.331 | 1.00 | 50.45 | O |
| ATOM | 2371 | CB  | TYR | A | 308 | 46.083 | 42.684 | 18.162 | 1.00 | 51.43 | C |
| ATOM | 2372 | CG  | TYR | A | 308 | 46.675 | 42.460 | 19.532 | 1.00 | 52.65 | C |
| ATOM | 2373 | CD1 | TYR | A | 308 | 45.925 | 42.712 | 20.674 | 1.00 | 52.95 | C |
| ATOM | 2374 | CD2 | TYR | A | 308 | 47.948 | 41.912 | 19.685 | 1.00 | 53.42 | C |
| ATOM | 2375 | CE1 | TYR | A | 308 | 46.435 | 42.472 | 21.925 | 1.00 | 54.01 | C |
| ATOM | 2376 | CE2 | TYR | A | 308 | 48.467 | 41.662 | 20.937 | 1.00 | 54.33 | C |
| ATOM | 2377 | CZ  | TYR | A | 308 | 47.703 | 41.949 | 22.058 | 1.00 | 54.84 | C |
| ATOM | 2378 | OH  | TYR | A | 308 | 48.189 | 41.714 | 23.323 | 1.00 | 56.45 | O |
| ATOM | 2379 | N   | PRO | A | 309 | 43.496 | 42.186 | 16.290 | 1.00 | 48.69 | N |
| ATOM | 2380 | CA  | PRO | A | 309 | 42.789 | 42.696 | 17.474 | 1.00 | 47.07 | C |
| ATOM | 2381 | C   | PRO | A | 309 | 42.127 | 41.586 | 18.280 | 1.00 | 44.55 | C |
| ATOM | 2382 | O   | PRO | A | 309 | 41.782 | 40.555 | 17.728 | 1.00 | 45.01 | O |
| ATOM | 2383 | CB  | PRO | A | 309 | 41.720 | 43.606 | 16.869 | 1.00 | 47.45 | C |
| ATOM | 2384 | CG  | PRO | A | 309 | 41.420 | 42.978 | 15.508 | 1.00 | 48.43 | C |
| ATOM | 2385 | CD  | PRO | A | 309 | 42.701 | 42.336 | 15.056 | 1.00 | 48.78 | C |
| ATOM | 2386 | N   | LEU | A | 310 | 41.967 | 41.790 | 19.577 | 1.00 | 41.78 | N |
| ATOM | 2387 | CA  | LEU | A | 310 | 41.344 | 40.781 | 20.427 | 1.00 | 39.59 | C |
| ATOM | 2388 | C   | LEU | A | 310 | 39.858 | 40.652 | 20.133 | 1.00 | 37.52 | C |
| ATOM | 2389 | O   | LEU | A | 310 | 39.171 | 41.655 | 19.923 | 1.00 | 38.11 | O |
| ATOM | 2390 | CB  | LEU | A | 310 | 41.499 | 41.174 | 21.893 | 1.00 | 39.43 | C |
| ATOM | 2391 | CG  | LEU | A | 310 | 42.527 | 40.468 | 22.784 | 1.00 | 38.86 | C |
| ATOM | 2392 | CD1 | LEU | A | 310 | 43.799 | 40.123 | 22.092 | 1.00 | 37.07 | C |
| ATOM | 2393 | CD2 | LEU | A | 310 | 42.799 | 41.326 | 24.000 | 1.00 | 38.37 | C |
| ATOM | 2394 | N   | LYS | A | 311 | 39.361 | 39.425 | 20.141 | 1.00 | 34.45 | N |
| ATOM | 2395 | CA  | LYS | A | 311 | 37.932 | 39.180 | 20.001 | 1.00 | 32.51 | C |
| ATOM | 2396 | C   | LYS | A | 311 | 37.144 | 39.537 | 21.257 | 1.00 | 30.59 | C |
| ATOM | 2397 | O   | LYS | A | 311 | 37.675 | 39.546 | 22.375 | 1.00 | 28.88 | O |
| ATOM | 2398 | CB  | LYS | A | 311 | 37.674 | 37.736 | 19.652 | 1.00 | 32.87 | C |
| ATOM | 2399 | N   | ALA | A | 312 | 35.853 | 39.786 | 21.057 | 1.00 | 28.39 | N |
| ATOM | 2400 | CA  | ALA | A | 312 | 34.991 | 40.141 | 22.155 | 1.00 | 27.14 | C |
| ATOM | 2401 | C   | ALA | A | 312 | 35.110 | 39.121 | 23.260 | 1.00 | 26.12 | C |
| ATOM | 2402 | O   | ALA | A | 312 | 35.274 | 39.509 | 24.411 | 1.00 | 24.47 | O |
| ATOM | 2403 | CB  | ALA | A | 312 | 33.552 | 40.323 | 21.710 | 1.00 | 26.63 | C |
| ATOM | 2404 | N   | HIS | A | 313 | 35.126 | 37.830 | 22.910 | 1.00 | 25.90 | N |
| ATOM | 2405 | CA  | HIS | A | 313 | 35.106 | 36.796 | 23.932 | 1.00 | 25.82 | C |
| ATOM | 2406 | C   | HIS | A | 313 | 36.411 | 36.749 | 24.690 | 1.00 | 25.03 | C |
| ATOM | 2407 | O   | HIS | A | 313 | 36.447 | 36.323 | 25.825 | 1.00 | 24.89 | O |
| ATOM | 2408 | CB  | HIS | A | 313 | 34.724 | 35.406 | 23.368 | 1.00 | 27.19 | C |
| ATOM | 2409 | CG  | HIS | A | 313 | 35.788 | 34.773 | 22.535 | 1.00 | 29.47 | C |
| ATOM | 2410 | ND1 | HIS | A | 313 | 35.963 | 35.078 | 21.198 | 1.00 | 34.94 | N |
| ATOM | 2411 | CD2 | HIS | A | 313 | 36.753 | 33.880 | 22.847 | 1.00 | 33.69 | C |
| ATOM | 2412 | CE1 | HIS | A | 313 | 37.006 | 34.411 | 20.730 | 1.00 | 35.11 | C |
| ATOM | 2413 | NE2 | HIS | A | 313 | 37.495 | 33.665 | 21.705 | 1.00 | 35.57 | N |
| ATOM | 2414 | N   | GLN | A | 314 | 37.491 | 37.185 | 24.072 | 1.00 | 24.60 | N |
| ATOM | 2415 | CA  | GLN | A | 314 | 38.764 | 37.226 | 24.753 | 1.00 | 24.57 | C |
| ATOM | 2416 | C   | GLN | A | 314 | 38.776 | 38.352 | 25.813 | 1.00 | 24.74 | C |
| ATOM | 2417 | O   | GLN | A | 314 | 39.371 | 38.201 | 26.881 | 1.00 | 24.48 | O |
| ATOM | 2418 | CB  | GLN | A | 314 | 39.898 | 37.420 | 23.745 | 1.00 | 24.79 | C |
| ATOM | 2419 | CG  | GLN | A | 314 | 40.067 | 36.241 | 22.794 | 1.00 | 26.08 | C |
| ATOM | 2420 | CD  | GLN | A | 314 | 41.109 | 36.488 | 21.730 | 1.00 | 27.10 | C |
| ATOM | 2421 | OE1 | GLN | A | 314 | 41.013 | 37.450 | 20.949 | 1.00 | 27.68 | O |
| ATOM | 2422 | NE2 | GLN | A | 314 | 42.123 | 35.629 | 21.699 | 1.00 | 29.52 | N |
| ATOM | 2423 | N   | LYS | A | 315 | 38.115 | 39.462 | 25.506 | 1.00 | 23.99 | N |
| ATOM | 2424 | CA  | LYS | A | 315 | 37.983 | 40.545 | 26.454 | 1.00 | 24.95 | C |
| ATOM | 2425 | C   | LYS | A | 315 | 37.099 | 40.114 | 27.622 | 1.00 | 24.32 | C |
| ATOM | 2426 | O   | LYS | A | 315 | 37.345 | 40.491 | 28.765 | 1.00 | 22.87 | O |
| ATOM | 2427 | CB  | LYS | A | 315 | 37.408 | 41.783 | 25.785 | 1.00 | 25.11 | C |
| ATOM | 2428 | CG  | LYS | A | 315 | 38.403 | 42.449 | 24.874 | 1.00 | 29.28 | C |
| ATOM | 2429 | CD  | LYS | A | 315 | 37.821 | 43.693 | 24.226 | 1.00 | 34.17 | C |
| ATOM | 2430 | CE  | LYS | A | 315 | 38.844 | 44.360 | 23.332 | 1.00 | 37.47 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2431 | NZ  | LYS | A | 315 | 38.206 | 45.270 | 22.318 | 1.00 | 41.38 | N |
| ATOM | 2432 | N   | VAL | A | 316 | 36.079 | 39.314 | 27.330 | 1.00 | 23.78 | N |
| ATOM | 2433 | CA  | VAL | A | 316 | 35.258 | 38.796 | 28.396 | 1.00 | 23.67 | C |
| ATOM | 2434 | C   | VAL | A | 316 | 36.138 | 37.937 | 29.329 | 1.00 | 23.61 | C |
| ATOM | 2435 | O   | VAL | A | 316 | 36.094 | 38.075 | 30.558 | 1.00 | 22.63 | O |
| ATOM | 2436 | CB  | VAL | A | 316 | 34.092 | 37.961 | 27.873 | 1.00 | 23.67 | C |
| ATOM | 2437 | CG1 | VAL | A | 316 | 33.315 | 37.370 | 29.037 | 1.00 | 23.53 | C |
| ATOM | 2438 | CG2 | VAL | A | 316 | 33.159 | 38.816 | 27.005 | 1.00 | 23.69 | C |
| ATOM | 2439 | N   | ALA | A | 317 | 36.940 | 37.065 | 28.732 | 1.00 | 22.51 | N |
| ATOM | 2440 | CA  | ALA | A | 317 | 37.834 | 36.207 | 29.507 | 1.00 | 22.28 | C |
| ATOM | 2441 | C   | ALA | A | 317 | 38.730 | 37.067 | 30.391 | 1.00 | 21.32 | C |
| ATOM | 2442 | O   | ALA | A | 317 | 38.926 | 36.783 | 31.556 | 1.00 | 21.45 | O |
| ATOM | 2443 | CB  | ALA | A | 317 | 38.680 | 35.325 | 28.574 | 1.00 | 21.87 | C |
| ATOM | 2444 | N   | ILE | A | 318 | 39.220 | 38.153 | 29.834 | 1.00 | 20.92 | N |
| ATOM | 2445 | CA  | ILE | A | 318 | 40.091 | 39.053 | 30.574 | 1.00 | 21.36 | C |
| ATOM | 2446 | C   | ILE | A | 318 | 39.375 | 39.662 | 31.784 | 1.00 | 21.54 | C |
| ATOM | 2447 | O   | ILE | A | 318 | 39.930 | 39.697 | 32.895 | 1.00 | 20.69 | O |
| ATOM | 2448 | CB  | ILE | A | 318 | 40.650 | 40.153 | 29.646 | 1.00 | 21.19 | C |
| ATOM | 2449 | CG1 | ILE | A | 318 | 41.664 | 39.560 | 28.670 | 1.00 | 21.41 | C |
| ATOM | 2450 | CG2 | ILE | A | 318 | 41.315 | 41.267 | 30.461 | 1.00 | 21.05 | C |
| ATOM | 2451 | CD1 | ILE | A | 318 | 42.217 | 40.569 | 27.663 | 1.00 | 21.73 | C |
| ATOM | 2452 | N   | MET | A | 319 | 38.146 | 40.122 | 31.569 | 1.00 | 21.31 | N |
| ATOM | 2453 | CA  | MET | A | 319 | 37.400 | 40.774 | 32.632 | 1.00 | 21.99 | C |
| ATOM | 2454 | C   | MET | A | 319 | 37.094 | 39.787 | 33.748 | 1.00 | 22.21 | C |
| ATOM | 2455 | O   | MET | A | 319 | 37.219 | 40.114 | 34.937 | 1.00 | 23.25 | O |
| ATOM | 2456 | CB  | MET | A | 319 | 36.133 | 41.446 | 32.108 | 1.00 | 21.66 | C |
| ATOM | 2457 | CG  | MET | A | 319 | 36.369 | 42.703 | 31.233 | 1.00 | 21.49 | C |
| ATOM | 2458 | SD  | MET | A | 319 | 34.787 | 43.525 | 30.787 | 1.00 | 23.05 | S |
| ATOM | 2459 | CE  | MET | A | 319 | 34.192 | 42.395 | 29.453 | 1.00 | 22.63 | C |
| ATOM | 2460 | N   | ARG | A | 320 | 36.736 | 38.568 | 33.379 | 1.00 | 21.99 | N |
| ATOM | 2461 | CA  | ARG | A | 320 | 36.492 | 37.544 | 34.383 | 1.00 | 21.57 | C |
| ATOM | 2462 | C   | ARG | A | 320 | 37.750 | 37.319 | 35.223 | 1.00 | 21.22 | C |
| ATOM | 2463 | O   | ARG | A | 320 | 37.669 | 37.210 | 36.439 | 1.00 | 21.65 | O |
| ATOM | 2464 | CB  | ARG | A | 320 | 36.083 | 36.237 | 33.726 | 1.00 | 20.79 | C |
| ATOM | 2465 | CG  | ARG | A | 320 | 34.702 | 36.243 | 33.014 | 1.00 | 22.36 | C |
| ATOM | 2466 | CD  | ARG | A | 320 | 34.300 | 34.857 | 32.452 | 1.00 | 21.24 | C |
| ATOM | 2467 | NE  | ARG | A | 320 | 34.147 | 33.910 | 33.558 | 1.00 | 21.37 | N |
| ATOM | 2468 | CZ  | ARG | A | 320 | 33.148 | 33.957 | 34.423 | 1.00 | 21.73 | C |
| ATOM | 2469 | NH1 | ARG | A | 320 | 32.196 | 34.869 | 34.308 | 1.00 | 22.69 | N |
| ATOM | 2470 | NH2 | ARG | A | 320 | 33.100 | 33.109 | 35.425 | 1.00 | 23.33 | N |
| ATOM | 2471 | N   | ASN | A | 321 | 38.908 | 37.216 | 34.571 | 1.00 | 21.35 | N |
| ATOM | 2472 | CA  | ASN | A | 321 | 40.159 | 36.947 | 35.282 | 1.00 | 21.20 | C |
| ATOM | 2473 | C   | ASN | A | 321 | 40.510 | 38.078 | 36.239 | 1.00 | 21.02 | C |
| ATOM | 2474 | O   | ASN | A | 321 | 40.958 | 37.828 | 37.364 | 1.00 | 21.80 | O |
| ATOM | 2475 | CB  | ASN | A | 321 | 41.314 | 36.648 | 34.311 | 1.00 | 21.07 | C |
| ATOM | 2476 | CG  | ASN | A | 321 | 41.263 | 35.209 | 33.752 | 1.00 | 22.81 | C |
| ATOM | 2477 | OD1 | ASN | A | 321 | 40.821 | 34.306 | 34.431 | 1.00 | 23.88 | O |
| ATOM | 2478 | ND2 | ASN | A | 321 | 41.713 | 35.018 | 32.521 | 1.00 | 20.59 | N |
| ATOM | 2479 | N   | ILE | A | 322 | 40.336 | 39.320 | 35.802 | 1.00 | 20.31 | N |
| ATOM | 2480 | CA  | ILE | A | 322 | 40.611 | 40.447 | 36.683 | 1.00 | 19.83 | C |
| ATOM | 2481 | C   | ILE | A | 322 | 39.721 | 40.344 | 37.918 | 1.00 | 19.45 | C |
| ATOM | 2482 | O   | ILE | A | 322 | 40.178 | 40.531 | 39.037 | 1.00 | 18.04 | O |
| ATOM | 2483 | CB  | ILE | A | 322 | 40.327 | 41.775 | 35.980 | 1.00 | 20.01 | C |
| ATOM | 2484 | CG1 | ILE | A | 322 | 41.320 | 42.009 | 34.849 | 1.00 | 21.62 | C |
| ATOM | 2485 | CG2 | ILE | A | 322 | 40.351 | 42.930 | 36.989 | 1.00 | 20.64 | C |
| ATOM | 2486 | CD1 | ILE | A | 322 | 42.782 | 41.987 | 35.278 | 1.00 | 23.99 | C |
| ATOM | 2487 | N   | GLU | A | 323 | 38.444 | 40.035 | 37.716 | 1.00 | 18.87 | N |
| ATOM | 2488 | CA  | GLU | A | 323 | 37.533 | 39.940 | 38.841 | 1.00 | 19.15 | C |
| ATOM | 2489 | C   | GLU | A | 323 | 37.964 | 38.845 | 39.781 | 1.00 | 19.09 | C |
| ATOM | 2490 | O   | GLU | A | 323 | 37.997 | 39.044 | 40.980 | 1.00 | 19.36 | O |
| ATOM | 2491 | CB  | GLU | A | 323 | 36.095 | 39.721 | 38.366 | 1.00 | 19.19 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2492 | CG  | GLU | A | 323 | 35.478 | 40.987 | 37.787 | 1.00 | 19.24 | C |
| ATOM | 2493 | CD  | GLU | A | 323 | 34.096 | 40.764 | 37.189 | 1.00 | 17.51 | C |
| ATOM | 2494 | OE1 | GLU | A | 323 | 33.140 | 40.470 | 37.922 | 1.00 | 17.44 | O |
| ATOM | 2495 | OE2 | GLU | A | 323 | 33.982 | 40.901 | 35.974 | 1.00 | 16.60 | O |
| ATOM | 2496 | N   | LYS | A | 324 | 38.357 | 37.711 | 39.227 | 1.00 | 19.47 | N |
| ATOM | 2497 | CA  | LYS | A | 324 | 38.781 | 36.570 | 40.037 | 1.00 | 20.33 | C |
| ATOM | 2498 | C   | LYS | A | 324 | 40.040 | 36.869 | 40.839 | 1.00 | 20.67 | C |
| ATOM | 2499 | O   | LYS | A | 324 | 40.090 | 36.562 | 42.023 | 1.00 | 20.56 | O |
| ATOM | 2500 | CB  | LYS | A | 324 | 39.040 | 35.334 | 39.172 | 1.00 | 20.11 | C |
| ATOM | 2501 | CG  | LYS | A | 324 | 37.803 | 34.678 | 38.572 | 1.00 | 20.73 | C |
| ATOM | 2502 | CD  | LYS | A | 324 | 38.238 | 33.413 | 37.761 | 1.00 | 21.68 | C |
| ATOM | 2503 | CE  | LYS | A | 324 | 37.117 | 32.866 | 36.857 | 1.00 | 22.30 | C |
| ATOM | 2504 | NZ  | LYS | A | 324 | 37.534 | 31.609 | 36.153 | 1.00 | 19.72 | N |
| ATOM | 2505 | N   | MET | A | 325 | 41.045 | 37.456 | 40.194 | 1.00 | 21.37 | N |
| ATOM | 2506 | CA  | MET | A | 325 | 42.305 | 37.782 | 40.860 | 1.00 | 22.78 | C |
| ATOM | 2507 | C   | MET | A | 325 | 42.106 | 38.789 | 41.990 | 1.00 | 22.78 | C |
| ATOM | 2508 | O   | MET | A | 325 | 42.734 | 38.694 | 43.047 | 1.00 | 22.48 | O |
| ATOM | 2509 | CB  | MET | A | 325 | 43.308 | 38.369 | 39.865 | 1.00 | 23.14 | C |
| ATOM | 2510 | CG  | MET | A | 325 | 43.964 | 37.359 | 38.978 | 1.00 | 27.30 | C |
| ATOM | 2511 | SD  | MET | A | 325 | 44.699 | 38.147 | 37.511 | 1.00 | 35.72 | S |
| ATOM | 2512 | CE  | MET | A | 325 | 45.804 | 39.221 | 38.338 | 1.00 | 36.16 | C |
| ATOM | 2513 | N   | LEU | A | 326 | 41.248 | 39.765 | 41.752 | 1.00 | 23.21 | N |
| ATOM | 2514 | CA  | LEU | A | 326 | 40.977 | 40.795 | 42.751 | 1.00 | 24.47 | C |
| ATOM | 2515 | C   | LEU | A | 326 | 40.307 | 40.195 | 43.969 | 1.00 | 24.48 | C |
| ATOM | 2516 | O   | LEU | A | 326 | 40.659 | 40.500 | 45.083 | 1.00 | 24.21 | O |
| ATOM | 2517 | CB  | LEU | A | 326 | 40.087 | 41.863 | 42.159 | 1.00 | 24.63 | C |
| ATOM | 2518 | CG  | LEU | A | 326 | 40.618 | 43.282 | 41.988 | 1.00 | 27.80 | C |
| ATOM | 2519 | CD1 | LEU | A | 326 | 42.135 | 43.441 | 42.036 | 1.00 | 28.29 | C |
| ATOM | 2520 | CD2 | LEU | A | 326 | 40.038 | 43.820 | 40.682 | 1.00 | 28.01 | C |
| ATOM | 2521 | N   | GLY | A | 327 | 39.350 | 39.314 | 43.726 | 1.00 | 25.29 | N |
| ATOM | 2522 | CA  | GLY | A | 327 | 38.663 | 38.608 | 44.782 | 1.00 | 25.73 | C |
| ATOM | 2523 | C   | GLY | A | 327 | 39.644 | 37.854 | 45.638 | 1.00 | 25.86 | C |
| ATOM | 2524 | O   | GLY | A | 327 | 39.597 | 37.931 | 46.863 | 1.00 | 25.83 | O |
| ATOM | 2525 | N   | GLU | A | 328 | 40.556 | 37.137 | 45.002 | 1.00 | 26.02 | N |
| ATOM | 2526 | CA  | GLU | A | 328 | 41.558 | 36.397 | 45.762 | 1.00 | 26.93 | C |
| ATOM | 2527 | C   | GLU | A | 328 | 42.557 | 37.306 | 46.480 | 1.00 | 25.70 | C |
| ATOM | 2528 | O   | GLU | A | 328 | 42.883 | 37.070 | 47.635 | 1.00 | 24.67 | O |
| ATOM | 2529 | CB  | GLU | A | 328 | 42.293 | 35.423 | 44.853 | 1.00 | 27.76 | C |
| ATOM | 2530 | CG  | GLU | A | 328 | 41.403 | 34.282 | 44.375 | 1.00 | 31.57 | C |
| ATOM | 2531 | CD  | GLU | A | 328 | 41.635 | 32.992 | 45.146 | 1.00 | 37.39 | C |
| ATOM | 2532 | OE1 | GLU | A | 328 | 42.048 | 33.058 | 46.335 | 1.00 | 41.34 | O |
| ATOM | 2533 | OE2 | GLU | A | 328 | 41.430 | 31.902 | 44.552 | 1.00 | 42.69 | O |
| ATOM | 2534 | N   | ALA | A | 329 | 43.024 | 38.356 | 45.816 | 1.00 | 25.20 | N |
| ATOM | 2535 | CA  | ALA | A | 329 | 44.031 | 39.219 | 46.433 | 1.00 | 25.42 | C |
| ATOM | 2536 | C   | ALA | A | 329 | 43.475 | 40.039 | 47.582 | 1.00 | 25.67 | C |
| ATOM | 2537 | O   | ALA | A | 329 | 44.141 | 40.247 | 48.570 | 1.00 | 25.92 | O |
| ATOM | 2538 | CB  | ALA | A | 329 | 44.670 | 40.109 | 45.409 | 1.00 | 25.31 | C |
| ATOM | 2539 | N   | LEU | A | 330 | 42.241 | 40.496 | 47.467 | 1.00 | 26.51 | N |
| ATOM | 2540 | CA  | LEU | A | 330 | 41.656 | 41.306 | 48.529 | 1.00 | 27.12 | C |
| ATOM | 2541 | C   | LEU | A | 330 | 41.156 | 40.453 | 49.677 | 1.00 | 27.74 | C |
| ATOM | 2542 | O   | LEU | A | 330 | 40.845 | 40.959 | 50.748 | 1.00 | 27.62 | O |
| ATOM | 2543 | CB  | LEU | A | 330 | 40.517 | 42.138 | 47.984 | 1.00 | 27.19 | C |
| ATOM | 2544 | CG  | LEU | A | 330 | 40.966 | 43.131 | 46.915 | 1.00 | 27.69 | C |
| ATOM | 2545 | CD1 | LEU | A | 330 | 39.747 | 43.661 | 46.211 | 1.00 | 28.15 | C |
| ATOM | 2546 | CD2 | LEU | A | 330 | 41.774 | 44.271 | 47.525 | 1.00 | 27.60 | C |
| ATOM | 2547 | N   | GLY | A | 331 | 41.054 | 39.154 | 49.434 | 1.00 | 28.45 | N |
| ATOM | 2548 | CA  | GLY | A | 331 | 40.637 | 38.222 | 50.457 | 1.00 | 29.04 | C |
| ATOM | 2549 | C   | GLY | A | 331 | 39.154 | 38.239 | 50.748 | 1.00 | 29.16 | C |
| ATOM | 2550 | O   | GLY | A | 331 | 38.698 | 37.505 | 51.615 | 1.00 | 29.67 | O |
| ATOM | 2551 | N   | ASN | A | 332 | 38.409 | 39.088 | 50.052 | 1.00 | 29.16 | N |
| ATOM | 2552 | CA  | ASN | A | 332 | 36.973 | 39.190 | 50.243 | 1.00 | 29.38 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2553 | C   | ASN | A | 332 | 36.342 | 39.718 | 48.958 | 1.00 | 28.80 | C |
| ATOM | 2554 | O   | ASN | A | 332 | 36.579 | 40.847 | 48.570 | 1.00 | 28.58 | O |
| ATOM | 2555 | CB  | ASN | A | 332 | 36.662 | 40.123 | 51.413 | 1.00 | 29.68 | C |
| ATOM | 2556 | CG  | ASN | A | 332 | 35.181 | 40.214 | 51.702 | 1.00 | 31.38 | C |
| ATOM | 2557 | OD1 | ASN | A | 332 | 34.368 | 39.630 | 50.991 | 1.00 | 35.54 | O |
| ATOM | 2558 | ND2 | ASN | A | 332 | 34.820 | 40.944 | 52.751 | 1.00 | 33.23 | N |
| ATOM | 2559 | N   | PRO | A | 333 | 35.504 | 38.922 | 48.325 | 1.00 | 28.45 | N |
| ATOM | 2560 | CA  | PRO | A | 333 | 34.944 | 39.288 | 47.025 | 1.00 | 28.38 | C |
| ATOM | 2561 | C   | PRO | A | 333 | 34.094 | 40.534 | 47.093 | 1.00 | 28.04 | C |
| ATOM | 2562 | O   | PRO | A | 333 | 33.913 | 41.187 | 46.073 | 1.00 | 28.11 | O |
| ATOM | 2563 | CB  | PRO | A | 333 | 34.071 | 38.093 | 46.640 | 1.00 | 28.23 | C |
| ATOM | 2564 | CG  | PRO | A | 333 | 34.203 | 37.097 | 47.701 | 1.00 | 29.36 | C |
| ATOM | 2565 | CD  | PRO | A | 333 | 34.999 | 37.641 | 48.822 | 1.00 | 28.91 | C |
| ATOM | 2566 | N   | GLN | A | 334 | 33.556 | 40.844 | 48.262 | 1.00 | 27.75 | N |
| ATOM | 2567 | CA  | GLN | A | 334 | 32.727 | 42.033 | 48.400 | 1.00 | 28.08 | C |
| ATOM | 2568 | C   | GLN | A | 334 | 33.582 | 43.282 | 48.300 | 1.00 | 26.62 | C |
| ATOM | 2569 | O   | GLN | A | 334 | 33.064 | 44.365 | 48.086 | 1.00 | 26.31 | O |
| ATOM | 2570 | CB  | GLN | A | 334 | 31.857 | 41.989 | 49.686 | 1.00 | 28.89 | C |
| ATOM | 2571 | CG  | GLN | A | 334 | 30.594 | 41.090 | 49.459 | 1.00 | 32.52 | C |
| ATOM | 2572 | CD  | GLN | A | 334 | 29.523 | 41.114 | 50.556 | 1.00 | 36.22 | C |
| ATOM | 2573 | OE1 | GLN | A | 334 | 29.500 | 42.004 | 51.421 | 1.00 | 39.82 | O |
| ATOM | 2574 | NE2 | GLN | A | 334 | 28.612 | 40.127 | 50.503 | 1.00 | 38.24 | N |
| ATOM | 2575 | N   | GLU | A | 335 | 34.894 | 43.138 | 48.414 | 1.00 | 25.23 | N |
| ATOM | 2576 | CA  | GLU | A | 335 | 35.763 | 44.290 | 48.269 | 1.00 | 24.55 | C |
| ATOM | 2577 | C   | GLU | A | 335 | 36.090 | 44.584 | 46.790 | 1.00 | 22.95 | C |
| ATOM | 2578 | O   | GLU | A | 335 | 36.691 | 45.597 | 46.475 | 1.00 | 21.47 | O |
| ATOM | 2579 | CB  | GLU | A | 335 | 37.038 | 44.091 | 49.088 | 1.00 | 25.61 | C |
| ATOM | 2580 | CG  | GLU | A | 335 | 36.820 | 44.189 | 50.599 | 1.00 | 29.47 | C |
| ATOM | 2581 | CD  | GLU | A | 335 | 38.115 | 44.280 | 51.369 | 1.00 | 34.49 | C |
| ATOM | 2582 | OE1 | GLU | A | 335 | 38.964 | 45.124 | 51.004 | 1.00 | 39.50 | O |
| ATOM | 2583 | OE2 | GLU | A | 335 | 38.288 | 43.521 | 52.350 | 1.00 | 40.05 | O |
| ATOM | 2584 | N   | VAL | A | 336 | 35.654 | 43.722 | 45.877 | 1.00 | 21.52 | N |
| ATOM | 2585 | CA  | VAL | A | 336 | 35.993 | 43.898 | 44.458 | 1.00 | 20.69 | C |
| ATOM | 2586 | C   | VAL | A | 336 | 35.422 | 45.176 | 43.855 | 1.00 | 19.97 | C |
| ATOM | 2587 | O   | VAL | A | 336 | 36.134 | 45.949 | 43.239 | 1.00 | 19.57 | O |
| ATOM | 2588 | CB  | VAL | A | 336 | 35.594 | 42.683 | 43.653 | 1.00 | 20.59 | C |
| ATOM | 2589 | CG1 | VAL | A | 336 | 35.746 | 42.933 | 42.179 | 1.00 | 21.20 | C |
| ATOM | 2590 | CG2 | VAL | A | 336 | 36.467 | 41.513 | 44.067 | 1.00 | 21.28 | C |
| ATOM | 2591 | N   | GLY | A | 337 | 34.146 | 45.421 | 44.080 | 1.00 | 19.82 | N |
| ATOM | 2592 | CA  | GLY | A | 337 | 33.492 | 46.598 | 43.568 | 1.00 | 19.66 | C |
| ATOM | 2593 | C   | GLY | A | 337 | 34.130 | 47.906 | 43.981 | 1.00 | 19.56 | C |
| ATOM | 2594 | O   | GLY | A | 337 | 34.510 | 48.693 | 43.131 | 1.00 | 19.35 | O |
| ATOM | 2595 | N   | PRO | A | 338 | 34.202 | 48.162 | 45.278 | 1.00 | 19.93 | N |
| ATOM | 2596 | CA  | PRO | A | 338 | 34.846 | 49.383 | 45.790 | 1.00 | 19.88 | C |
| ATOM | 2597 | C   | PRO | A | 338 | 36.272 | 49.631 | 45.254 | 1.00 | 19.22 | C |
| ATOM | 2598 | O   | PRO | A | 338 | 36.591 | 50.758 | 44.908 | 1.00 | 18.43 | O |
| ATOM | 2599 | CB  | PRO | A | 338 | 34.830 | 49.191 | 47.316 | 1.00 | 19.61 | C |
| ATOM | 2600 | CG  | PRO | A | 338 | 33.625 | 48.380 | 47.555 | 1.00 | 20.33 | C |
| ATOM | 2601 | CD  | PRO | A | 338 | 33.579 | 47.367 | 46.359 | 1.00 | 20.75 | C |
| ATOM | 2602 | N   | LEU | A | 339 | 37.107 | 48.612 | 45.171 | 1.00 | 19.21 | N |
| ATOM | 2603 | CA  | LEU | A | 339 | 38.416 | 48.814 | 44.566 | 1.00 | 19.65 | C |
| ATOM | 2604 | C   | LEU | A | 339 | 38.283 | 49.219 | 43.081 | 1.00 | 19.35 | C |
| ATOM | 2605 | O   | LEU | A | 339 | 38.927 | 50.188 | 42.621 | 1.00 | 17.91 | O |
| ATOM | 2606 | CB  | LEU | A | 339 | 39.279 | 47.570 | 44.693 | 1.00 | 20.38 | C |
| ATOM | 2607 | CG  | LEU | A | 339 | 40.745 | 47.814 | 44.291 | 1.00 | 21.96 | C |
| ATOM | 2608 | CD1 | LEU | A | 339 | 41.681 | 47.151 | 45.220 | 1.00 | 25.12 | C |
| ATOM | 2609 | CD2 | LEU | A | 339 | 40.991 | 47.293 | 42.899 | 1.00 | 22.54 | C |
| ATOM | 2610 | N   | LEU | A | 340 | 37.420 | 48.512 | 42.345 | 1.00 | 19.18 | N |
| ATOM | 2611 | CA  | LEU | A | 340 | 37.231 | 48.821 | 40.928 | 1.00 | 19.26 | C |
| ATOM | 2612 | C   | LEU | A | 340 | 36.764 | 50.260 | 40.746 | 1.00 | 19.52 | C |
| ATOM | 2613 | O   | LEU | A | 340 | 37.306 | 50.989 | 39.893 | 1.00 | 18.71 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2614 | CB  | LEU | A | 340 | 36.260 | 47.857 | 40.273 | 1.00 | 19.85 | C |
| ATOM | 2615 | CG  | LEU | A | 340 | 36.823 | 46.470 | 39.960 | 1.00 | 21.77 | C |
| ATOM | 2616 | CD1 | LEU | A | 340 | 35.745 | 45.671 | 39.299 | 1.00 | 22.81 | C |
| ATOM | 2617 | CD2 | LEU | A | 340 | 38.088 | 46.539 | 39.072 | 1.00 | 21.14 | C |
| ATOM | 2618 | N   | ASN | A | 341 | 35.798 | 50.676 | 41.570 | 1.00 | 19.12 | N |
| ATOM | 2619 | CA  | ASN | A | 341 | 35.296 | 52.052 | 41.536 | 1.00 | 20.43 | C |
| ATOM | 2620 | C   | ASN | A | 341 | 36.367 | 53.086 | 41.865 | 1.00 | 19.90 | C |
| ATOM | 2621 | O   | ASN | A | 341 | 36.474 | 54.110 | 41.206 | 1.00 | 19.81 | O |
| ATOM | 2622 | CB  | ASN | A | 341 | 34.090 | 52.232 | 42.485 | 1.00 | 20.40 | C |
| ATOM | 2623 | CG  | ASN | A | 341 | 32.814 | 51.659 | 41.898 | 1.00 | 24.06 | C |
| ATOM | 2624 | OD1 | ASN | A | 341 | 32.390 | 52.073 | 40.829 | 1.00 | 31.36 | O |
| ATOM | 2625 | ND2 | ASN | A | 341 | 32.229 | 50.666 | 42.561 | 1.00 | 25.82 | N |
| ATOM | 2626 | N   | THR | A | 342 | 37.129 | 52.812 | 42.912 | 1.00 | 19.43 | N |
| ATOM | 2627 | CA  | THR | A | 342 | 38.227 | 53.664 | 43.305 | 1.00 | 19.71 | C |
| ATOM | 2628 | C   | THR | A | 342 | 39.230 | 53.781 | 42.154 | 1.00 | 19.45 | C |
| ATOM | 2629 | O   | THR | A | 342 | 39.739 | 54.859 | 41.893 | 1.00 | 19.23 | O |
| ATOM | 2630 | CB  | THR | A | 342 | 38.873 | 53.073 | 44.555 | 1.00 | 20.44 | C |
| ATOM | 2631 | OG1 | THR | A | 342 | 38.030 | 53.322 | 45.700 | 1.00 | 21.13 | O |
| ATOM | 2632 | CG2 | THR | A | 342 | 40.208 | 53.756 | 44.874 | 1.00 | 20.71 | C |
| ATOM | 2633 | N   | MET | A | 343 | 39.464 | 52.691 | 41.427 | 1.00 | 19.49 | N |
| ATOM | 2634 | CA  | MET | A | 343 | 40.381 | 52.723 | 40.287 | 1.00 | 19.90 | C |
| ATOM | 2635 | C   | MET | A | 343 | 39.932 | 53.649 | 39.164 | 1.00 | 19.94 | C |
| ATOM | 2636 | O   | MET | A | 343 | 40.775 | 54.344 | 38.567 | 1.00 | 18.43 | O |
| ATOM | 2637 | CB  | MET | A | 343 | 40.543 | 51.347 | 39.664 | 1.00 | 19.92 | C |
| ATOM | 2638 | CG  | MET | A | 343 | 41.701 | 50.556 | 40.115 | 1.00 | 23.07 | C |
| ATOM | 2639 | SD  | MET | A | 343 | 42.163 | 49.194 | 38.959 | 1.00 | 24.93 | S |
| ATOM | 2640 | CE  | MET | A | 343 | 41.013 | 48.220 | 39.315 | 1.00 | 27.48 | C |
| ATOM | 2641 | N   | ILE | A | 344 | 38.629 | 53.643 | 38.837 | 1.00 | 20.84 | N |
| ATOM | 2642 | CA  | ILE | A | 344 | 38.159 | 54.412 | 37.679 | 1.00 | 21.51 | C |
| ATOM | 2643 | C   | ILE | A | 344 | 37.624 | 55.800 | 37.918 | 1.00 | 21.46 | C |
| ATOM | 2644 | O   | ILE | A | 344 | 37.751 | 56.639 | 37.018 | 1.00 | 21.65 | O |
| ATOM | 2645 | CB  | ILE | A | 344 | 37.089 | 53.641 | 36.805 | 1.00 | 22.58 | C |
| ATOM | 2646 | CG1 | ILE | A | 344 | 35.714 | 53.723 | 37.435 | 1.00 | 24.65 | C |
| ATOM | 2647 | CG2 | ILE | A | 344 | 37.506 | 52.220 | 36.555 | 1.00 | 23.63 | C |
| ATOM | 2648 | CD1 | ILE | A | 344 | 34.635 | 53.407 | 36.511 | 1.00 | 28.35 | C |
| ATOM | 2649 | N   | LYS | A | 345 | 37.009 | 56.092 | 39.062 | 1.00 | 21.48 | N |
| ATOM | 2650 | CA  | LYS | A | 345 | 36.410 | 57.433 | 39.154 | 1.00 | 22.11 | C |
| ATOM | 2651 | C   | LYS | A | 345 | 37.382 | 58.569 | 39.127 | 1.00 | 20.79 | C |
| ATOM | 2652 | O   | LYS | A | 345 | 38.380 | 58.614 | 39.863 | 1.00 | 20.06 | O |
| ATOM | 2653 | CB  | LYS | A | 345 | 35.405 | 57.656 | 40.279 | 1.00 | 23.49 | C |
| ATOM | 2654 | CG  | LYS | A | 345 | 35.497 | 56.838 | 41.473 | 1.00 | 28.03 | C |
| ATOM | 2655 | CD  | LYS | A | 345 | 34.120 | 56.183 | 41.683 | 1.00 | 30.07 | C |
| ATOM | 2656 | CE  | LYS | A | 345 | 33.282 | 56.986 | 42.624 | 1.00 | 32.44 | C |
| ATOM | 2657 | NZ  | LYS | A | 345 | 33.859 | 56.977 | 43.982 | 1.00 | 36.32 | N |
| ATOM | 2658 | N   | GLY | A | 346 | 37.062 | 59.501 | 38.243 | 1.00 | 19.28 | N |
| ATOM | 2659 | CA  | GLY | A | 346 | 37.911 | 60.636 | 38.013 | 1.00 | 18.60 | C |
| ATOM | 2660 | C   | GLY | A | 346 | 39.222 | 60.254 | 37.350 | 1.00 | 17.41 | C |
| ATOM | 2661 | O   | GLY | A | 346 | 40.090 | 61.079 | 37.229 | 1.00 | 18.04 | O |
| ATOM | 2662 | N   | ARG | A | 347 | 39.353 | 59.024 | 36.898 | 1.00 | 17.62 | N |
| ATOM | 2663 | CA  | ARG | A | 347 | 40.616 | 58.563 | 36.297 | 1.00 | 17.91 | C |
| ATOM | 2664 | C   | ARG | A | 347 | 40.415 | 57.992 | 34.874 | 1.00 | 18.08 | C |
| ATOM | 2665 | O   | ARG | A | 347 | 41.108 | 58.395 | 33.938 | 1.00 | 17.06 | O |
| ATOM | 2666 | CB  | ARG | A | 347 | 41.284 | 57.532 | 37.213 | 1.00 | 17.51 | C |
| ATOM | 2667 | CG  | ARG | A | 347 | 41.719 | 58.081 | 38.592 | 1.00 | 15.94 | C |
| ATOM | 2668 | CD  | ARG | A | 347 | 43.179 | 57.649 | 38.985 | 1.00 | 19.49 | C |
| ATOM | 2669 | NE  | ARG | A | 347 | 43.165 | 56.242 | 38.980 | 1.00 | 18.58 | N |
| ATOM | 2670 | CZ  | ARG | A | 347 | 44.048 | 55.405 | 38.518 | 1.00 | 14.88 | C |
| ATOM | 2671 | NH1 | ARG | A | 347 | 45.271 | 55.726 | 38.085 | 1.00 | 17.47 | N |
| ATOM | 2672 | NH2 | ARG | A | 347 | 43.678 | 54.158 | 38.611 | 1.00 | 11.18 | N |
| ATOM | 2673 | N   | TYR | A | 348 | 39.450 | 57.091 | 34.732 | 1.00 | 18.81 | N |
| ATOM | 2674 | CA  | TYR | A | 348 | 39.098 | 56.480 | 33.444 | 1.00 | 20.50 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2675 | C   | TYR | A | 348 | 37.637 | 56.691 | 33.036 | 1.00 | 22.07 | C |
| ATOM | 2676 | O   | TYR | A | 348 | 37.233 | 56.236 | 31.978 | 1.00 | 22.11 | O |
| ATOM | 2677 | CB  | TYR | A | 348 | 39.311 | 54.963 | 33.478 | 1.00 | 19.77 | C |
| ATOM | 2678 | CG  | TYR | A | 348 | 40.753 | 54.545 | 33.561 | 1.00 | 20.36 | C |
| ATOM | 2679 | CD1 | TYR | A | 348 | 41.540 | 54.483 | 32.422 | 1.00 | 19.91 | C |
| ATOM | 2680 | CD2 | TYR | A | 348 | 41.335 | 54.225 | 34.780 | 1.00 | 18.20 | C |
| ATOM | 2681 | CE1 | TYR | A | 348 | 42.859 | 54.099 | 32.489 | 1.00 | 19.81 | C |
| ATOM | 2682 | CE2 | TYR | A | 348 | 42.662 | 53.841 | 34.863 | 1.00 | 19.47 | C |
| ATOM | 2683 | CZ  | TYR | A | 348 | 43.425 | 53.785 | 33.711 | 1.00 | 19.43 | C |
| ATOM | 2684 | OH  | TYR | A | 348 | 44.742 | 53.414 | 33.773 | 1.00 | 15.61 | O |
| ATOM | 2685 | N   | ASN | A | 349 | 36.820 | 57.344 | 33.850 | 1.00 | 24.37 | N |
| ATOM | 2686 | CA  | ASN | A | 349 | 35.414 | 57.472 | 33.456 | 1.00 | 26.66 | C |
| ATOM | 2687 | C   | ASN | A | 349 | 34.941 | 58.854 | 33.092 | 1.00 | 28.03 | C |
| ATOM | 2688 | O   | ASN | A | 349 | 35.663 | 59.847 | 32.992 | 1.00 | 27.79 | O |
| ATOM | 2689 | CB  | ASN | A | 349 | 34.498 | 56.919 | 34.518 | 1.00 | 26.23 | C |
| ATOM | 2690 | CG  | ASN | A | 349 | 34.463 | 57.764 | 35.748 | 1.00 | 27.89 | C |
| ATOM | 2691 | OD1 | ASN | A | 349 | 35.247 | 58.718 | 35.927 | 1.00 | 27.38 | O |
| ATOM | 2692 | ND2 | ASN | A | 349 | 33.545 | 57.409 | 36.645 | 1.00 | 32.46 | N |
| ATOM | 2693 | OXT | ASN | A | 349 | 33.736 | 58.963 | 32.900 | 1.00 | 32.44 | O |
| TER  | 2694 |     | ASN | A | 349 |        |        |        |      |       |   |
| ATOM | 2695 | N   | LEU | S | 795 | 45.819 | 35.786 | 30.984 | 1.00 | 36.91 | N |
| ATOM | 2696 | CA  | LEU | S | 795 | 44.711 | 36.756 | 31.250 | 1.00 | 37.26 | C |
| ATOM | 2697 | C   | LEU | S | 795 | 43.553 | 36.418 | 30.323 | 1.00 | 37.49 | C |
| ATOM | 2698 | O   | LEU | S | 795 | 42.391 | 36.451 | 30.712 | 1.00 | 36.90 | O |
| ATOM | 2699 | CB  | LEU | S | 795 | 45.183 | 38.186 | 31.044 | 1.00 | 37.26 | C |
| ATOM | 2700 | CG  | LEU | S | 795 | 44.683 | 39.204 | 32.074 | 1.00 | 37.32 | C |
| ATOM | 2701 | CD1 | LEU | S | 795 | 44.775 | 38.671 | 33.479 | 1.00 | 37.34 | C |
| ATOM | 2702 | CD2 | LEU | S | 795 | 45.479 | 40.493 | 32.006 | 1.00 | 37.95 | C |
| ATOM | 2703 | N   | THR | S | 796 | 43.907 | 36.155 | 29.076 | 1.00 | 38.07 | N |
| ATOM | 2704 | CA  | THR | S | 796 | 43.029 | 35.548 | 28.076 | 1.00 | 39.17 | C |
| ATOM | 2705 | C   | THR | S | 796 | 42.608 | 34.088 | 28.347 | 1.00 | 38.93 | C |
| ATOM | 2706 | O   | THR | S | 796 | 41.784 | 33.533 | 27.622 | 1.00 | 39.51 | O |
| ATOM | 2707 | CB  | THR | S | 796 | 43.750 | 35.628 | 26.705 | 1.00 | 39.45 | C |
| ATOM | 2708 | OG1 | THR | S | 796 | 43.287 | 34.597 | 25.850 | 1.00 | 41.87 | O |
| ATOM | 2709 | CG2 | THR | S | 796 | 45.232 | 35.275 | 26.824 | 1.00 | 40.14 | C |
| ATOM | 2710 | N   | SER | S | 797 | 43.154 | 33.451 | 29.369 | 1.00 | 38.98 | N |
| ATOM | 2711 | CA  | SER | S | 797 | 42.770 | 32.067 | 29.654 | 1.00 | 39.24 | C |
| ATOM | 2712 | C   | SER | S | 797 | 41.370 | 31.981 | 30.274 | 1.00 | 39.32 | C |
| ATOM | 2713 | O   | SER | S | 797 | 40.901 | 32.905 | 30.939 | 1.00 | 38.28 | O |
| ATOM | 2714 | CB  | SER | S | 797 | 43.775 | 31.398 | 30.574 | 1.00 | 38.98 | C |
| ATOM | 2715 | OG  | SER | S | 797 | 43.613 | 31.884 | 31.891 | 1.00 | 40.40 | O |
| ATOM | 2716 | N   | TYR | S | 798 | 40.713 | 30.851 | 30.059 | 1.00 | 39.93 | N |
| ATOM | 2717 | CA  | TYR | S | 798 | 39.345 | 30.682 | 30.515 | 1.00 | 40.53 | C |
| ATOM | 2718 | C   | TYR | S | 798 | 39.088 | 29.350 | 31.183 | 1.00 | 39.72 | C |
| ATOM | 2719 | O   | TYR | S | 798 | 39.797 | 28.383 | 30.958 | 1.00 | 39.72 | O |
| ATOM | 2720 | CB  | TYR | S | 798 | 38.377 | 30.881 | 29.351 | 1.00 | 41.28 | C |
| ATOM | 2721 | CG  | TYR | S | 798 | 38.524 | 29.939 | 28.171 | 1.00 | 44.57 | C |
| ATOM | 2722 | CD1 | TYR | S | 798 | 39.574 | 30.071 | 27.261 | 1.00 | 47.13 | C |
| ATOM | 2723 | CD2 | TYR | S | 798 | 37.574 | 28.953 | 27.932 | 1.00 | 47.85 | C |
| ATOM | 2724 | CE1 | TYR | S | 798 | 39.692 | 29.219 | 26.163 | 1.00 | 48.81 | C |
| ATOM | 2725 | CE2 | TYR | S | 798 | 37.680 | 28.094 | 26.833 | 1.00 | 50.32 | C |
| ATOM | 2726 | CZ  | TYR | S | 798 | 38.744 | 28.229 | 25.955 | 1.00 | 49.97 | C |
| ATOM | 2727 | OH  | TYR | S | 798 | 38.835 | 27.387 | 24.866 | 1.00 | 49.58 | O |
| ATOM | 2728 | N   | ASP | S | 799 | 38.051 | 29.306 | 32.005 | 1.00 | 39.16 | N |
| ATOM | 2729 | CA  | ASP | S | 799 | 37.676 | 28.076 | 32.690 | 1.00 | 38.61 | C |
| ATOM | 2730 | C   | ASP | S | 799 | 36.588 | 27.391 | 31.868 | 1.00 | 37.26 | C |
| ATOM | 2731 | O   | ASP | S | 799 | 36.468 | 27.657 | 30.671 | 1.00 | 36.81 | O |
| ATOM | 2732 | CB  | ASP | S | 799 | 37.186 | 28.399 | 34.105 | 1.00 | 39.29 | C |
| ATOM | 2733 | CG  | ASP | S | 799 | 37.303 | 27.223 | 35.048 | 1.00 | 40.55 | C |
| ATOM | 2734 | OD1 | ASP | S | 799 | 36.767 | 26.128 | 34.756 | 1.00 | 41.68 | O |
| ATOM | 2735 | OD2 | ASP | S | 799 | 37.913 | 27.319 | 36.121 | 1.00 | 45.38 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2736 | N   | CYS | S | 800 | 35.795 | 26.517 | 32.486 | 1.00 | 35.61 | N |
| ATOM | 2737 | CA  | CYS | S | 800 | 34.781 | 25.787 | 31.732 | 1.00 | 34.66 | C |
| ATOM | 2738 | C   | CYS | S | 800 | 33.439 | 25.714 | 32.450 | 1.00 | 34.03 | C |
| ATOM | 2739 | O   | CYS | S | 800 | 32.749 | 24.708 | 32.388 | 1.00 | 33.81 | O |
| ATOM | 2740 | CB  | CYS | S | 800 | 35.274 | 24.380 | 31.423 | 1.00 | 34.32 | C |
| ATOM | 2741 | SG  | CYS | S | 800 | 35.538 | 23.392 | 32.911 | 1.00 | 33.88 | S |
| ATOM | 2742 | N   | GLU | S | 801 | 33.051 | 26.792 | 33.101 | 1.00 | 33.69 | N |
| ATOM | 2743 | CA  | GLU | S | 801 | 31.808 | 26.803 | 33.859 | 1.00 | 33.94 | C |
| ATOM | 2744 | C   | GLU | S | 801 | 30.551 | 26.980 | 32.991 | 1.00 | 33.69 | C |
| ATOM | 2745 | O   | GLU | S | 801 | 30.520 | 27.739 | 32.012 | 1.00 | 32.67 | O |
| ATOM | 2746 | CB  | GLU | S | 801 | 31.886 | 27.877 | 34.942 | 1.00 | 34.03 | C |
| ATOM | 2747 | CG  | GLU | S | 801 | 33.128 | 27.703 | 35.818 | 1.00 | 36.03 | C |
| ATOM | 2748 | CD  | GLU | S | 801 | 33.095 | 28.557 | 37.065 | 1.00 | 36.15 | C |
| ATOM | 2749 | OE1 | GLU | S | 801 | 32.408 | 28.163 | 38.013 | 1.00 | 35.62 | O |
| ATOM | 2750 | OE2 | GLU | S | 801 | 33.751 | 29.619 | 37.090 | 1.00 | 38.69 | O |
| ATOM | 2751 | N   | VAL | S | 802 | 29.519 | 26.242 | 33.377 | 1.00 | 33.95 | N |
| ATOM | 2752 | CA  | VAL | S | 802 | 28.244 | 26.223 | 32.691 | 1.00 | 33.82 | C |
| ATOM | 2753 | C   | VAL | S | 802 | 27.137 | 26.148 | 33.735 | 1.00 | 34.17 | C |
| ATOM | 2754 | O   | VAL | S | 802 | 27.408 | 25.928 | 34.908 | 1.00 | 33.56 | O |
| ATOM | 2755 | CB  | VAL | S | 802 | 28.139 | 24.972 | 31.781 | 1.00 | 33.63 | C |
| ATOM | 2756 | CG1 | VAL | S | 802 | 29.263 | 24.948 | 30.753 | 1.00 | 32.61 | C |
| ATOM | 2757 | CG2 | VAL | S | 802 | 28.165 | 23.682 | 32.624 | 1.00 | 33.77 | C |
| ATOM | 2758 | N   | ASN | S | 803 | 25.887 | 26.304 | 33.300 | 1.00 | 35.05 | N |
| ATOM | 2759 | CA  | ASN | S | 803 | 24.745 | 26.222 | 34.204 | 1.00 | 35.82 | C |
| ATOM | 2760 | C   | ASN | S | 803 | 24.457 | 24.784 | 34.642 | 1.00 | 37.45 | C |
| ATOM | 2761 | O   | ASN | S | 803 | 23.379 | 24.241 | 34.387 | 1.00 | 37.12 | O |
| ATOM | 2762 | CB  | ASN | S | 803 | 23.490 | 26.836 | 33.573 | 1.00 | 35.36 | C |
| ATOM | 2763 | CG  | ASN | S | 803 | 23.548 | 28.344 | 33.506 | 1.00 | 33.54 | C |
| ATOM | 2764 | OD1 | ASN | S | 803 | 24.605 | 28.941 | 33.685 | 1.00 | 32.05 | O |
| ATOM | 2765 | ND2 | ASN | S | 803 | 22.414 | 28.967 | 33.230 | 1.00 | 29.41 | N |
| ATOM | 2766 | N   | ALA | S | 804 | 25.442 | 24.187 | 35.298 | 1.00 | 39.28 | N |
| ATOM | 2767 | CA  | ALA | S | 804 | 25.340 | 22.846 | 35.855 | 1.00 | 41.13 | C |
| ATOM | 2768 | C   | ALA | S | 804 | 26.566 | 22.620 | 36.734 | 1.00 | 42.43 | C |
| ATOM | 2769 | O   | ALA | S | 804 | 27.638 | 23.153 | 36.464 | 1.00 | 42.47 | O |
| ATOM | 2770 | CB  | ALA | S | 804 | 25.277 | 21.791 | 34.762 | 1.00 | 41.08 | C |
| ATOM | 2771 | N   | PRO | S | 805 | 26.410 | 21.830 | 37.786 | 1.00 | 44.47 | N |
| ATOM | 2772 | CA  | PRO | S | 805 | 27.527 | 21.527 | 38.697 | 1.00 | 45.68 | C |
| ATOM | 2773 | C   | PRO | S | 805 | 28.568 | 20.620 | 38.053 | 1.00 | 46.82 | C |
| ATOM | 2774 | O   | PRO | S | 805 | 28.273 | 19.918 | 37.092 | 1.00 | 47.40 | O |
| ATOM | 2775 | CB  | PRO | S | 805 | 26.847 | 20.783 | 39.854 | 1.00 | 45.66 | C |
| ATOM | 2776 | CG  | PRO | S | 805 | 25.588 | 20.206 | 39.261 | 1.00 | 45.01 | C |
| ATOM | 2777 | CD  | PRO | S | 805 | 25.161 | 21.146 | 38.177 | 1.00 | 44.63 | C |
| ATOM | 2778 | N   | ILE | S | 806 | 29.770 | 20.613 | 38.605 | 1.00 | 48.31 | N |
| ATOM | 2779 | CA  | ILE | S | 806 | 30.847 | 19.766 | 38.098 | 1.00 | 49.34 | C |
| ATOM | 2780 | C   | ILE | S | 806 | 30.661 | 18.323 | 38.555 | 1.00 | 49.57 | C |
| ATOM | 2781 | O   | ILE | S | 806 | 29.992 | 18.063 | 39.560 | 1.00 | 50.13 | O |
| ATOM | 2782 | CB  | ILE | S | 806 | 32.215 | 20.311 | 38.574 | 1.00 | 49.85 | C |
| ATOM | 2783 | CG1 | ILE | S | 806 | 32.410 | 20.058 | 40.074 | 1.00 | 50.64 | C |
| ATOM | 2784 | CG2 | ILE | S | 806 | 32.327 | 21.816 | 38.250 | 1.00 | 50.45 | C |
| ATOM | 2785 | CD1 | ILE | S | 806 | 33.724 | 20.605 | 40.624 | 1.00 | 51.43 | C |
| ATOM | 2786 | N   | LEU | S | 813 | 29.871 | 8.315  | 36.218 | 1.00 | 46.23 | N |
| ATOM | 2787 | CA  | LEU | S | 813 | 30.588 | 8.788  | 35.034 | 1.00 | 46.32 | C |
| ATOM | 2788 | C   | LEU | S | 813 | 29.685 | 9.635  | 34.140 | 1.00 | 45.87 | C |
| ATOM | 2789 | O   | LEU | S | 813 | 28.463 | 9.511  | 34.185 | 1.00 | 45.43 | O |
| ATOM | 2790 | CB  | LEU | S | 813 | 31.166 | 7.606  | 34.243 | 1.00 | 46.25 | C |
| ATOM | 2791 | CG  | LEU | S | 813 | 32.057 | 6.663  | 35.059 | 1.00 | 46.61 | C |
| ATOM | 2792 | CD1 | LEU | S | 813 | 32.444 | 5.423  | 34.230 | 1.00 | 46.51 | C |
| ATOM | 2793 | CD2 | LEU | S | 813 | 33.292 | 7.406  | 35.579 | 1.00 | 45.98 | C |
| ATOM | 2794 | N   | GLN | S | 814 | 30.309 | 10.503 | 33.351 | 1.00 | 45.81 | N |
| ATOM | 2795 | CA  | GLN | S | 814 | 29.595 | 11.400 | 32.446 | 1.00 | 45.92 | C |
| ATOM | 2796 | C   | GLN | S | 814 | 30.497 | 11.838 | 31.296 | 1.00 | 45.66 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2797 | O   | GLN | S | 814 | 31.706 | 11.626 | 31.329 | 1.00 | 45.05 | O |
| ATOM | 2798 | CB  | GLN | S | 814 | 29.123 | 12.643 | 33.198 | 1.00 | 46.09 | C |
| ATOM | 2799 | CG  | GLN | S | 814 | 30.265 | 13.531 | 33.696 | 1.00 | 47.32 | C |
| ATOM | 2800 | CD  | GLN | S | 814 | 29.781 | 14.722 | 34.520 | 1.00 | 49.22 | C |
| ATOM | 2801 | OE1 | GLN | S | 814 | 29.165 | 14.541 | 35.569 | 1.00 | 50.40 | O |
| ATOM | 2802 | NE2 | GLN | S | 814 | 30.070 | 15.937 | 34.053 | 1.00 | 49.45 | N |
| ATOM | 2803 | N   | GLY | S | 815 | 29.898 | 12.476 | 30.294 | 1.00 | 45.88 | N |
| ATOM | 2804 | CA  | GLY | S | 815 | 30.621 | 12.956 | 29.135 | 1.00 | 45.84 | C |
| ATOM | 2805 | C   | GLY | S | 815 | 31.426 | 11.863 | 28.462 | 1.00 | 46.13 | C |
| ATOM | 2806 | O   | GLY | S | 815 | 30.968 | 10.732 | 28.339 | 1.00 | 45.49 | O |
| ATOM | 2807 | N   | GLU | S | 816 | 32.633 | 12.216 | 28.035 | 1.00 | 46.94 | N |
| ATOM | 2808 | CA  | GLU | S | 816 | 33.548 | 11.285 | 27.382 | 1.00 | 48.03 | C |
| ATOM | 2809 | C   | GLU | S | 816 | 33.721 | 9.994  | 28.186 | 1.00 | 48.62 | C |
| ATOM | 2810 | O   | GLU | S | 816 | 33.823 | 8.910  | 27.614 | 1.00 | 48.54 | O |
| ATOM | 2811 | CB  | GLU | S | 816 | 34.920 | 11.948 | 27.184 | 1.00 | 48.06 | C |
| ATOM | 2812 | CG  | GLU | S | 816 | 35.783 | 11.312 | 26.102 | 1.00 | 48.93 | C |
| ATOM | 2813 | CD  | GLU | S | 816 | 37.189 | 11.887 | 26.062 | 1.00 | 49.77 | C |
| ATOM | 2814 | OE1 | GLU | S | 816 | 38.031 | 11.413 | 26.848 | 1.00 | 50.86 | O |
| ATOM | 2815 | OE2 | GLU | S | 816 | 37.457 | 12.802 | 25.247 | 1.00 | 49.55 | O |
| ATOM | 2816 | N   | GLU | S | 817 | 33.737 | 10.112 | 29.509 | 1.00 | 49.67 | N |
| ATOM | 2817 | CA  | GLU | S | 817 | 33.947 | 8.957  | 30.373 | 1.00 | 50.75 | C |
| ATOM | 2818 | C   | GLU | S | 817 | 32.786 | 7.982  | 30.309 | 1.00 | 51.10 | C |
| ATOM | 2819 | O   | GLU | S | 817 | 32.989 | 6.771  | 30.278 | 1.00 | 51.12 | O |
| ATOM | 2820 | CB  | GLU | S | 817 | 34.164 | 9.406  | 31.815 | 1.00 | 50.97 | C |
| ATOM | 2821 | CG  | GLU | S | 817 | 35.476 | 10.140 | 32.032 | 1.00 | 52.22 | C |
| ATOM | 2822 | CD  | GLU | S | 817 | 35.395 | 11.637 | 31.764 | 1.00 | 54.47 | C |
| ATOM | 2823 | OE1 | GLU | S | 817 | 34.289 | 12.166 | 31.489 | 1.00 | 55.57 | O |
| ATOM | 2824 | OE2 | GLU | S | 817 | 36.456 | 12.296 | 31.833 | 1.00 | 56.41 | O |
| ATOM | 2825 | N   | LEU | S | 818 | 31.572 | 8.521  | 30.295 | 1.00 | 51.81 | N |
| ATOM | 2826 | CA  | LEU | S | 818 | 30.376 | 7.706  | 30.204 | 1.00 | 52.37 | C |
| ATOM | 2827 | C   | LEU | S | 818 | 30.399 | 6.929  | 28.901 | 1.00 | 53.14 | C |
| ATOM | 2828 | O   | LEU | S | 818 | 30.216 | 5.714  | 28.894 | 1.00 | 53.00 | O |
| ATOM | 2829 | CB  | LEU | S | 818 | 29.116 | 8.575  | 30.258 | 1.00 | 52.25 | C |
| ATOM | 2830 | CG  | LEU | S | 818 | 27.786 | 7.814  | 30.176 | 1.00 | 52.17 | C |
| ATOM | 2831 | CD1 | LEU | S | 818 | 27.661 | 6.836  | 31.335 | 1.00 | 52.37 | C |
| ATOM | 2832 | CD2 | LEU | S | 818 | 26.596 | 8.749  | 30.173 | 1.00 | 51.16 | C |
| ATOM | 2833 | N   | LEU | S | 819 | 30.660 | 7.643  | 27.809 | 1.00 | 54.00 | N |
| ATOM | 2834 | CA  | LEU | S | 819 | 30.623 | 7.068  | 26.465 | 1.00 | 54.73 | C |
| ATOM | 2835 | C   | LEU | S | 819 | 31.573 | 5.874  | 26.295 | 1.00 | 55.32 | C |
| ATOM | 2836 | O   | LEU | S | 819 | 31.171 | 4.823  | 25.794 | 1.00 | 55.08 | O |
| ATOM | 2837 | CB  | LEU | S | 819 | 30.929 | 8.162  | 25.426 | 1.00 | 54.66 | C |
| ATOM | 2838 | CG  | LEU | S | 819 | 30.838 | 7.789  | 23.942 | 1.00 | 54.90 | C |
| ATOM | 2839 | CD1 | LEU | S | 819 | 29.480 | 7.239  | 23.559 | 1.00 | 54.56 | C |
| ATOM | 2840 | CD2 | LEU | S | 819 | 31.170 | 8.997  | 23.088 | 1.00 | 55.68 | C |
| ATOM | 2841 | N   | ARG | S | 820 | 32.821 | 6.036  | 26.725 | 1.00 | 55.92 | N |
| ATOM | 2842 | CA  | ARG | S | 820 | 33.817 | 4.987  | 26.576 | 1.00 | 56.75 | C |
| ATOM | 2843 | C   | ARG | S | 820 | 33.488 | 3.762  | 27.428 | 1.00 | 56.92 | C |
| ATOM | 2844 | O   | ARG | S | 820 | 33.578 | 2.617  | 26.951 | 1.00 | 56.86 | O |
| ATOM | 2845 | CB  | ARG | S | 820 | 35.207 | 5.530  | 26.915 | 1.00 | 57.13 | C |
| ATOM | 2846 | CG  | ARG | S | 820 | 35.638 | 6.596  | 25.927 | 1.00 | 58.55 | C |
| ATOM | 2847 | CD  | ARG | S | 820 | 37.073 | 7.038  | 26.036 | 1.00 | 60.19 | C |
| ATOM | 2848 | NE  | ARG | S | 820 | 37.336 | 8.126  | 25.096 | 1.00 | 62.23 | N |
| ATOM | 2849 | CZ  | ARG | S | 820 | 38.465 | 8.831  | 25.039 | 1.00 | 64.08 | C |
| ATOM | 2850 | NH1 | ARG | S | 820 | 39.475 | 8.567  | 25.865 | 1.00 | 64.81 | N |
| ATOM | 2851 | NH2 | ARG | S | 820 | 38.586 | 9.805  | 24.142 | 1.00 | 64.58 | N |
| ATOM | 2852 | N   | ALA | S | 821 | 33.109 | 4.003  | 28.682 | 1.00 | 56.90 | N |
| ATOM | 2853 | CA  | ALA | S | 821 | 32.713 | 2.919  | 29.567 | 1.00 | 56.79 | C |
| ATOM | 2854 | C   | ALA | S | 821 | 31.611 | 2.106  | 28.880 | 1.00 | 56.74 | C |
| ATOM | 2855 | O   | ALA | S | 821 | 31.665 | 0.873  | 28.843 | 1.00 | 56.66 | O |
| ATOM | 2856 | CB  | ALA | S | 821 | 32.236 | 3.463  | 30.899 | 1.00 | 56.66 | C |
| ATOM | 2857 | N   | LEU | S | 822 | 30.629 | 2.806  | 28.317 | 1.00 | 56.51 | N |

|        |      |     |     |       |     |        |        |        |      |       |    |
|--------|------|-----|-----|-------|-----|--------|--------|--------|------|-------|----|
| ATOM   | 2858 | CA  | LEU | S     | 822 | 29.537 | 2.155  | 27.607 | 1.00 | 56.58 | C  |
| ATOM   | 2859 | C   | LEU | S     | 822 | 30.031 | 1.473  | 26.338 | 1.00 | 56.66 | C  |
| ATOM   | 2860 | O   | LEU | S     | 822 | 29.482 | 0.451  | 25.931 | 1.00 | 57.09 | O  |
| ATOM   | 2861 | CB  | LEU | S     | 822 | 28.451 | 3.167  | 27.250 | 1.00 | 56.48 | C  |
| ATOM   | 2862 | CG  | LEU | S     | 822 | 27.681 | 3.779  | 28.417 | 1.00 | 56.11 | C  |
| ATOM   | 2863 | CD1 | LEU | S     | 822 | 26.543 | 4.612  | 27.870 | 1.00 | 55.96 | C  |
| ATOM   | 2864 | CD2 | LEU | S     | 822 | 27.156 | 2.717  | 29.379 | 1.00 | 55.80 | C  |
| TER    | 2865 |     | LEU | S     | 822 |        |        |        |      |       |    |
| HETATM | 2866 | FE  | FE2 | A1350 |     | 23.313 | 27.671 | 28.779 | 1.00 | 22.12 | FE |
| HETATM | 2867 | C1  | AKG | A1351 |     | 22.355 | 25.315 | 27.747 | 1.00 | 25.61 | C  |
| HETATM | 2868 | O1  | AKG | A1351 |     | 23.449 | 25.880 | 27.756 | 1.00 | 27.58 | O  |
| HETATM | 2869 | O2  | AKG | A1351 |     | 22.172 | 24.103 | 27.197 | 1.00 | 27.99 | O  |
| HETATM | 2870 | C2  | AKG | A1351 |     | 21.128 | 25.999 | 28.365 | 1.00 | 24.14 | C  |
| HETATM | 2871 | O5  | AKG | A1351 |     | 21.211 | 27.117 | 28.854 | 1.00 | 23.66 | O  |
| HETATM | 2872 | C3  | AKG | A1351 |     | 19.829 | 25.231 | 28.280 | 1.00 | 23.46 | C  |
| HETATM | 2873 | C4  | AKG | A1351 |     | 18.717 | 25.967 | 29.008 | 1.00 | 22.15 | C  |
| HETATM | 2874 | C5  | AKG | A1351 |     | 17.351 | 25.435 | 28.649 | 1.00 | 23.90 | C  |
| HETATM | 2875 | O3  | AKG | A1351 |     | 17.136 | 24.674 | 27.706 | 1.00 | 23.27 | O  |
| HETATM | 2876 | O4  | AKG | A1351 |     | 16.353 | 25.844 | 29.406 | 1.00 | 25.34 | O  |
| HETATM | 2877 | S   | SO4 | A1352 |     | 0.196  | 25.255 | 43.681 | 1.00 | 83.69 | S  |
| HETATM | 2878 | O1  | SO4 | A1352 |     | 1.049  | 26.078 | 44.531 | 1.00 | 83.03 | O  |
| HETATM | 2879 | O2  | SO4 | A1352 |     | 1.028  | 24.391 | 42.840 | 1.00 | 82.84 | O  |
| HETATM | 2880 | O3  | SO4 | A1352 |     | -0.643 | 24.431 | 44.542 | 1.00 | 83.90 | O  |
| HETATM | 2881 | O4  | SO4 | A1352 |     | -0.630 | 26.114 | 42.830 | 1.00 | 82.82 | O  |
| HETATM | 2882 | S   | SO4 | A1353 |     | 1.937  | 28.607 | 29.759 | 1.00 | 80.69 | S  |
| HETATM | 2883 | O1  | SO4 | A1353 |     | 3.164  | 29.179 | 30.298 | 1.00 | 79.82 | O  |
| HETATM | 2884 | O2  | SO4 | A1353 |     | 2.228  | 27.552 | 28.793 | 1.00 | 79.89 | O  |
| HETATM | 2885 | O3  | SO4 | A1353 |     | 1.188  | 28.079 | 30.902 | 1.00 | 82.14 | O  |
| HETATM | 2886 | O4  | SO4 | A1353 |     | 1.145  | 29.630 | 29.081 | 1.00 | 81.49 | O  |
| HETATM | 2887 | O   | HOH | H     | 1   | 38.423 | 33.864 | 31.899 | 1.00 | 39.52 | O  |
| HETATM | 2888 | O   | HOH | H     | 2   | 38.025 | 25.366 | 29.554 | 1.00 | 64.59 | O  |
| HETATM | 2889 | O   | HOH | H     | 3   | 34.915 | 30.689 | 35.190 | 1.00 | 34.36 | O  |
| HETATM | 2890 | O   | HOH | H     | 4   | 20.482 | 27.037 | 33.306 | 1.00 | 55.20 | O  |
| HETATM | 2891 | O   | HOH | H     | 5   | 21.066 | 24.447 | 32.916 | 1.00 | 43.55 | O  |
| HETATM | 2892 | O   | HOH | H     | 6   | 29.978 | 24.394 | 35.721 | 1.00 | 43.81 | O  |
| HETATM | 2893 | O   | HOH | H     | 7   | 29.346 | 18.985 | 42.744 | 1.00 | 86.25 | O  |
| HETATM | 2894 | O   | HOH | H     | 8   | 35.530 | 13.904 | 24.157 | 1.00 | 42.65 | O  |
| HETATM | 2895 | O   | HOH | H     | 9   | 33.804 | -1.383 | 26.877 | 1.00 | 65.05 | O  |
| HETATM | 2896 | O   | HOH | Z     | 1   | 11.560 | 21.626 | 13.846 | 1.00 | 41.47 | O  |
| HETATM | 2897 | O   | HOH | Z     | 2   | 9.590  | 21.877 | 12.314 | 1.00 | 61.59 | O  |
| HETATM | 2898 | O   | HOH | Z     | 3   | 1.321  | 21.339 | 7.657  | 1.00 | 58.53 | O  |
| HETATM | 2899 | O   | HOH | Z     | 4   | 3.579  | 13.365 | 8.778  | 1.00 | 47.77 | O  |
| HETATM | 2900 | O   | HOH | Z     | 5   | 4.515  | 16.855 | 3.766  | 1.00 | 51.50 | O  |
| HETATM | 2901 | O   | HOH | Z     | 6   | 2.462  | 19.552 | 5.161  | 1.00 | 56.40 | O  |
| HETATM | 2902 | O   | HOH | Z     | 7   | 1.251  | 29.413 | 13.184 | 1.00 | 52.18 | O  |
| HETATM | 2903 | O   | HOH | Z     | 8   | 2.053  | 32.304 | 13.875 | 1.00 | 71.43 | O  |
| HETATM | 2904 | O   | HOH | Z     | 9   | 11.574 | 44.907 | 14.867 | 1.00 | 67.18 | O  |
| HETATM | 2905 | O   | HOH | Z     | 10  | 11.615 | 3.238  | 17.221 | 1.00 | 63.99 | O  |
| HETATM | 2906 | O   | HOH | Z     | 11  | 3.752  | 32.951 | 32.375 | 1.00 | 72.66 | O  |
| HETATM | 2907 | O   | HOH | Z     | 12  | 4.803  | 37.611 | 27.421 | 1.00 | 63.47 | O  |
| HETATM | 2908 | O   | HOH | Z     | 13  | 11.007 | 35.734 | 30.393 | 1.00 | 34.95 | O  |
| HETATM | 2909 | O   | HOH | Z     | 14  | 15.551 | 46.392 | 24.481 | 1.00 | 43.01 | O  |
| HETATM | 2910 | O   | HOH | Z     | 15  | 12.231 | 41.979 | 15.720 | 1.00 | 53.94 | O  |
| HETATM | 2911 | O   | HOH | Z     | 16  | 13.868 | 4.815  | 17.661 | 1.00 | 48.46 | O  |
| HETATM | 2912 | O   | HOH | Z     | 17  | 15.860 | 30.606 | 12.755 | 1.00 | 44.45 | O  |
| HETATM | 2913 | O   | HOH | Z     | 18  | 13.462 | 22.030 | 7.390  | 1.00 | 59.18 | O  |
| HETATM | 2914 | O   | HOH | Z     | 19  | 14.706 | 26.336 | 13.845 | 1.00 | 51.42 | O  |
| HETATM | 2915 | O   | HOH | Z     | 20  | 17.028 | 29.994 | 7.603  | 1.00 | 64.07 | O  |
| HETATM | 2916 | O   | HOH | Z     | 21  | 21.135 | 23.988 | 3.773  | 1.00 | 46.32 | O  |
| HETATM | 2917 | O   | HOH | Z     | 22  | 27.581 | 31.130 | 6.026  | 1.00 | 64.13 | O  |
| HETATM | 2918 | O   | HOH | Z     | 23  | 27.341 | 22.242 | 43.414 | 1.00 | 79.43 | O  |



|        |      |   |     |   |    |        |        |        |      |       |   |
|--------|------|---|-----|---|----|--------|--------|--------|------|-------|---|
| HETATM | 2919 | O | HOH | Z | 24 | 36.742 | 29.331 | 21.279 | 1.00 | 50.70 | O |
| HETATM | 2920 | O | HOH | Z | 25 | 30.029 | 33.533 | 9.206  | 1.00 | 50.33 | O |
| HETATM | 2921 | O | HOH | Z | 26 | 29.955 | 37.104 | 10.551 | 1.00 | 70.40 | O |
| HETATM | 2922 | O | HOH | Z | 27 | 18.215 | 15.129 | 13.036 | 1.00 | 37.33 | O |
| HETATM | 2923 | O | HOH | Z | 28 | 29.069 | 5.533  | 17.355 | 1.00 | 44.84 | O |
| HETATM | 2924 | O | HOH | Z | 29 | 18.941 | 14.771 | 16.383 | 1.00 | 31.41 | O |
| HETATM | 2925 | O | HOH | Z | 30 | 13.624 | 7.655  | 18.343 | 1.00 | 46.45 | O |
| HETATM | 2926 | O | HOH | Z | 31 | 5.649  | 12.667 | 27.758 | 1.00 | 44.15 | O |
| HETATM | 2927 | O | HOH | Z | 32 | 18.818 | 6.772  | 36.717 | 1.00 | 51.59 | O |
| HETATM | 2928 | O | HOH | Z | 33 | 7.620  | 14.589 | 19.463 | 1.00 | 50.93 | O |
| HETATM | 2929 | O | HOH | Z | 34 | 20.087 | 9.746  | 36.974 | 1.00 | 52.81 | O |
| HETATM | 2930 | O | HOH | Z | 35 | 21.912 | 13.173 | 44.511 | 1.00 | 59.64 | O |
| HETATM | 2931 | O | HOH | Z | 36 | 29.233 | 39.992 | 16.108 | 1.00 | 75.75 | O |
| HETATM | 2932 | O | HOH | Z | 37 | 33.785 | 44.067 | 25.671 | 1.00 | 62.06 | O |
| HETATM | 2933 | O | HOH | Z | 38 | 15.613 | 37.779 | 35.493 | 1.00 | 52.50 | O |
| HETATM | 2934 | O | HOH | Z | 39 | 8.070  | 38.292 | 35.056 | 1.00 | 60.61 | O |
| HETATM | 2935 | O | HOH | Z | 40 | 16.339 | 30.957 | 40.378 | 1.00 | 43.15 | O |
| HETATM | 2936 | O | HOH | Z | 41 | 28.116 | 27.147 | 37.617 | 1.00 | 59.20 | O |
| HETATM | 2937 | O | HOH | Z | 42 | 29.707 | 30.087 | 39.279 | 1.00 | 54.89 | O |
| HETATM | 2938 | O | HOH | Z | 43 | 28.116 | 24.509 | 42.048 | 1.00 | 63.13 | O |
| HETATM | 2939 | O | HOH | Z | 44 | 25.074 | 24.801 | 42.258 | 1.00 | 54.81 | O |
| HETATM | 2940 | O | HOH | Z | 45 | 33.873 | 31.493 | 39.077 | 1.00 | 45.97 | O |
| HETATM | 2941 | O | HOH | Z | 46 | 31.533 | 33.860 | 46.118 | 1.00 | 50.65 | O |
| HETATM | 2942 | O | HOH | Z | 47 | 13.319 | 35.957 | 31.390 | 1.00 | 44.72 | O |
| HETATM | 2943 | O | HOH | Z | 48 | 27.155 | 38.119 | 52.311 | 1.00 | 64.05 | O |
| HETATM | 2944 | O | HOH | Z | 49 | 24.587 | 38.767 | 49.612 | 1.00 | 50.58 | O |
| HETATM | 2945 | O | HOH | Z | 50 | 21.687 | 17.630 | 48.071 | 1.00 | 77.36 | O |
| HETATM | 2946 | O | HOH | Z | 51 | 21.437 | 14.872 | 40.880 | 1.00 | 60.20 | O |
| HETATM | 2947 | O | HOH | Z | 52 | 24.790 | 15.406 | 39.359 | 1.00 | 78.81 | O |
| HETATM | 2948 | O | HOH | Z | 53 | 23.347 | 17.356 | 36.625 | 1.00 | 52.48 | O |
| HETATM | 2949 | O | HOH | Z | 54 | 21.628 | 10.475 | 34.469 | 1.00 | 47.30 | O |
| HETATM | 2950 | O | HOH | Z | 55 | 18.013 | -1.527 | 33.036 | 1.00 | 61.93 | O |
| HETATM | 2951 | O | HOH | Z | 56 | 16.101 | -0.104 | 30.078 | 1.00 | 59.33 | O |
| HETATM | 2952 | O | HOH | Z | 57 | 26.268 | 5.539  | 16.988 | 1.00 | 38.42 | O |
| HETATM | 2953 | O | HOH | Z | 58 | 30.916 | 16.527 | 11.437 | 1.00 | 44.01 | O |
| HETATM | 2954 | O | HOH | Z | 59 | 32.683 | 13.953 | 20.664 | 1.00 | 50.04 | O |
| HETATM | 2955 | O | HOH | Z | 60 | 36.797 | 10.766 | 7.771  | 1.00 | 80.75 | O |
| HETATM | 2956 | O | HOH | Z | 61 | 33.878 | 26.222 | 17.133 | 1.00 | 45.23 | O |
| HETATM | 2957 | O | HOH | Z | 62 | 13.442 | 21.089 | 28.459 | 1.00 | 36.04 | O |
| HETATM | 2958 | O | HOH | Z | 63 | 3.999  | 21.370 | 30.471 | 1.00 | 47.33 | O |
| HETATM | 2959 | O | HOH | Z | 64 | 30.697 | 38.141 | 33.290 | 1.00 | 31.70 | O |
| HETATM | 2960 | O | HOH | Z | 65 | 26.005 | 26.456 | 26.227 | 1.00 | 28.76 | O |
| HETATM | 2961 | O | HOH | Z | 66 | 36.729 | 32.146 | 33.280 | 1.00 | 42.61 | O |
| HETATM | 2962 | O | HOH | Z | 67 | 35.846 | 25.574 | 27.896 | 1.00 | 34.95 | O |
| HETATM | 2963 | O | HOH | Z | 68 | 36.793 | 26.712 | 21.173 | 1.00 | 33.97 | O |
| HETATM | 2964 | O | HOH | Z | 69 | 17.427 | 17.022 | 18.148 | 1.00 | 31.28 | O |
| HETATM | 2965 | O | HOH | Z | 70 | 9.904  | 13.694 | 19.533 | 1.00 | 41.70 | O |
| HETATM | 2966 | O | HOH | Z | 71 | 5.361  | 16.931 | 22.051 | 1.00 | 43.04 | O |
| HETATM | 2967 | O | HOH | Z | 72 | 7.094  | 16.984 | 20.250 | 1.00 | 43.57 | O |
| HETATM | 2968 | O | HOH | Z | 73 | 6.562  | 22.961 | 22.902 | 1.00 | 42.74 | O |
| HETATM | 2969 | O | HOH | Z | 74 | 29.508 | 38.942 | 26.471 | 1.00 | 26.72 | O |
| HETATM | 2970 | O | HOH | Z | 75 | 30.732 | 39.209 | 19.135 | 1.00 | 37.64 | O |
| HETATM | 2971 | O | HOH | Z | 76 | 26.368 | 42.318 | 17.836 | 1.00 | 57.14 | O |
| HETATM | 2972 | O | HOH | Z | 77 | 27.688 | 44.616 | 31.257 | 1.00 | 30.61 | O |
| HETATM | 2973 | O | HOH | Z | 78 | 30.230 | 44.988 | 25.170 | 1.00 | 39.14 | O |
| HETATM | 2974 | O | HOH | Z | 79 | 27.780 | 48.720 | 30.030 | 1.00 | 38.89 | O |
| HETATM | 2975 | O | HOH | Z | 80 | 25.931 | 50.741 | 30.611 | 1.00 | 40.27 | O |
| HETATM | 2976 | O | HOH | Z | 81 | 18.521 | 38.529 | 36.775 | 1.00 | 43.87 | O |
| HETATM | 2977 | O | HOH | Z | 82 | 26.678 | 31.402 | 38.482 | 1.00 | 36.08 | O |
| HETATM | 2978 | O | HOH | Z | 83 | 30.586 | 30.409 | 36.592 | 1.00 | 32.57 | O |
| HETATM | 2979 | O | HOH | Z | 84 | 29.411 | 37.141 | 35.473 | 1.00 | 26.16 | O |



|        |      |      |      |      |      |        |        |        |      |       |   |
|--------|------|------|------|------|------|--------|--------|--------|------|-------|---|
| HETATM | 2980 | O    | HOH  | Z    | 85   | 19.821 | 31.713 | 33.874 | 1.00 | 34.80 | O |
| HETATM | 2981 | O    | HOH  | Z    | 86   | 19.420 | 36.322 | 33.379 | 1.00 | 32.92 | O |
| HETATM | 2982 | O    | HOH  | Z    | 87   | 21.063 | 42.853 | 40.110 | 1.00 | 41.23 | O |
| HETATM | 2983 | O    | HOH  | Z    | 88   | 17.544 | 37.859 | 32.276 | 1.00 | 35.87 | O |
| HETATM | 2984 | O    | HOH  | Z    | 89   | 9.230  | 41.082 | 35.833 | 1.00 | 51.41 | O |
| HETATM | 2985 | O    | HOH  | Z    | 90   | 9.313  | 43.744 | 27.890 | 1.00 | 70.60 | O |
| HETATM | 2986 | O    | HOH  | Z    | 91   | 12.728 | 42.598 | 26.938 | 1.00 | 40.87 | O |
| HETATM | 2987 | O    | HOH  | Z    | 92   | 15.113 | 37.993 | 32.591 | 1.00 | 35.55 | O |
| HETATM | 2988 | O    | HOH  | Z    | 93   | 10.676 | 48.283 | 31.613 | 1.00 | 62.24 | O |
| HETATM | 2989 | O    | HOH  | Z    | 94   | 15.611 | 44.853 | 34.883 | 1.00 | 32.72 | O |
| HETATM | 2990 | O    | HOH  | Z    | 95   | 15.874 | 51.836 | 39.217 | 1.00 | 66.58 | O |
| HETATM | 2991 | O    | HOH  | Z    | 96   | 15.796 | 47.224 | 39.264 | 1.00 | 52.95 | O |
| HETATM | 2992 | O    | HOH  | Z    | 97   | 26.624 | 53.557 | 28.816 | 1.00 | 69.05 | O |
| HETATM | 2993 | O    | HOH  | Z    | 98   | 15.381 | 50.418 | 22.170 | 1.00 | 36.68 | O |
| HETATM | 2994 | O    | HOH  | Z    | 99   | 15.121 | 55.730 | 27.489 | 1.00 | 51.35 | O |
| HETATM | 2995 | O    | HOH  | Z    | 100  | 18.542 | 56.170 | 28.175 | 1.00 | 58.02 | O |
| HETATM | 2996 | O    | HOH  | Z    | 101  | 23.731 | 46.355 | 19.907 | 1.00 | 39.06 | O |
| HETATM | 2997 | O    | HOH  | Z    | 102  | 16.618 | 46.781 | 22.039 | 1.00 | 33.91 | O |
| HETATM | 2998 | O    | HOH  | Z    | 103  | 26.585 | 40.624 | 15.634 | 1.00 | 69.17 | O |
| HETATM | 2999 | O    | HOH  | Z    | 104  | 12.758 | 29.333 | 13.489 | 1.00 | 35.42 | O |
| HETATM | 3000 | O    | HOH  | Z    | 105  | 10.886 | 19.245 | 14.132 | 1.00 | 51.89 | O |
| HETATM | 3001 | O    | HOH  | Z    | 106  | 19.776 | 18.049 | 13.245 | 1.00 | 33.88 | O |
| HETATM | 3002 | O    | HOH  | Z    | 107  | 14.725 | 18.642 | 12.190 | 1.00 | 40.50 | O |
| HETATM | 3003 | O    | HOH  | Z    | 108  | 27.783 | 27.681 | 24.556 | 1.00 | 27.24 | O |
| HETATM | 3004 | O    | HOH  | Z    | 109  | 35.999 | 32.896 | 30.270 | 1.00 | 41.19 | O |
| HETATM | 3005 | O    | HOH  | Z    | 110  | 30.237 | 36.282 | 26.881 | 1.00 | 28.77 | O |
| HETATM | 3006 | O    | HOH  | Z    | 111  | 32.759 | 34.258 | 19.346 | 1.00 | 47.40 | O |
| HETATM | 3007 | O    | HOH  | Z    | 112  | 27.418 | 30.315 | 25.756 | 1.00 | 27.70 | O |
| HETATM | 3008 | O    | HOH  | Z    | 113  | 16.248 | 36.360 | 29.657 | 1.00 | 34.03 | O |
| HETATM | 3009 | O    | HOH  | Z    | 114  | 7.438  | 31.072 | 24.792 | 1.00 | 43.13 | O |
| HETATM | 3010 | O    | HOH  | Z    | 115  | 7.743  | 30.565 | 27.379 | 1.00 | 39.83 | O |
| HETATM | 3011 | O    | HOH  | Z    | 116  | 5.158  | 19.080 | 24.012 | 1.00 | 45.77 | O |
| HETATM | 3012 | O    | HOH  | Z    | 117  | 6.366  | 24.013 | 25.459 | 1.00 | 41.84 | O |
| HETATM | 3013 | O    | HOH  | Z    | 118  | 42.594 | 37.813 | 18.527 | 1.00 | 64.57 | O |
| HETATM | 3014 | O    | HOH  | Z    | 119  | 42.361 | 44.340 | 19.742 | 1.00 | 59.24 | O |
| HETATM | 3015 | O    | HOH  | Z    | 120  | 34.674 | 39.749 | 17.782 | 1.00 | 53.99 | O |
| HETATM | 3016 | O    | HOH  | Z    | 121  | 33.762 | 37.015 | 20.310 | 1.00 | 39.85 | O |
| HETATM | 3017 | O    | HOH  | Z    | 122  | 33.121 | 39.446 | 33.667 | 1.00 | 30.35 | O |
| HETATM | 3018 | O    | HOH  | Z    | 123  | 37.674 | 29.865 | 38.229 | 1.00 | 64.32 | O |
| HETATM | 3019 | O    | HOH  | Z    | 124  | 38.677 | 34.824 | 42.977 | 1.00 | 44.37 | O |
| HETATM | 3020 | O    | HOH  | Z    | 125  | 41.375 | 43.570 | 51.489 | 1.00 | 52.41 | O |
| HETATM | 3021 | O    | HOH  | Z    | 126  | 31.947 | 40.559 | 44.192 | 1.00 | 38.39 | O |
| HETATM | 3022 | O    | HOH  | Z    | 127  | 39.124 | 57.396 | 42.134 | 1.00 | 27.12 | O |
| HETATM | 3023 | O    | HOH  | Z    | 128  | 41.949 | 60.812 | 33.590 | 1.00 | 49.78 | O |
| HETATM | 3024 | O    | HOH  | Z    | 129  | 46.835 | 53.394 | 32.063 | 1.00 | 33.50 | O |
| HETATM | 3025 | O    | HOH  | Z    | 130  | 37.841 | 55.408 | 29.621 | 1.00 | 45.14 | O |
| CONECT | 1482 | 2866 |      |      |      |        |        |        |      |       |   |
| CONECT | 1502 | 2866 |      |      |      |        |        |        |      |       |   |
| CONECT | 2171 | 2866 |      |      |      |        |        |        |      |       |   |
| CONECT | 2866 | 2871 | 2868 | 1482 | 2171 | 1502   |        |        |      |       |   |
| CONECT | 2867 | 2868 | 2869 | 2870 |      |        |        |        |      |       |   |
| CONECT | 2868 | 2867 | 2866 |      |      |        |        |        |      |       |   |
| CONECT | 2869 | 2867 |      |      |      |        |        |        |      |       |   |
| CONECT | 2870 | 2867 | 2871 | 2872 |      |        |        |        |      |       |   |
| CONECT | 2871 | 2866 | 2870 |      |      |        |        |        |      |       |   |
| CONECT | 2872 | 2870 | 2873 |      |      |        |        |        |      |       |   |
| CONECT | 2873 | 2872 | 2874 |      |      |        |        |        |      |       |   |
| CONECT | 2874 | 2873 | 2875 | 2876 |      |        |        |        |      |       |   |
| CONECT | 2875 | 2874 |      |      |      |        |        |        |      |       |   |
| CONECT | 2876 | 2874 |      |      |      |        |        |        |      |       |   |
| CONECT | 2877 | 2878 | 2879 | 2880 | 2881 |        |        |        |      |       |   |

CONNECT 2878 2877  
CONNECT 2879 2877  
CONNECT 2880 2877  
CONNECT 2881 2877  
CONNECT 2882 2883 2884 2885 2886  
CONNECT 2883 2882  
CONNECT 2884 2882  
CONNECT 2885 2882  
CONNECT 2886 2882  
MASTER 437 0 4 15 20 0 7 6 3023 2 24 31  
END

Structure 3

Below are the coordinates for structure 3 (the 2.5 Å structure of FIH:Zn(II):NOG:CAD):

```

HEADER      TRANSCRIPTION ACTIVATOR/INHIBITOR          12-AUG-02   1H2M
TITLE       FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE       2 FRAGMENT PEPTIDE
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND      3 SYNONYM: FIH1;
COMPND      4 CHAIN: A;
COMPND      5 ENGINEERED: YES;
COMPND      6 MOL_ID: 2;
COMPND      7 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND      8 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
COMPND      9 MEMBER OF PAS PROTEIN 1, MOP1, HIF1 ALPHA, HIF1A.
COMPND     10 CHAIN: S;
COMPND     11 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND     12 RESIDUES 775 - 826
SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE      3 ORGANISM_COMMON: HUMAN;
SOURCE      4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE      5 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE      6 EXPRESSION_SYSTEM_PLASMID: PET28A(+);
SOURCE      7 MOL_ID: 2;
SOURCE      8 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE      9 ORGANISM_COMMON: HUMAN;
SOURCE     10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE     11 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE     12 EXPRESSION_SYSTEM_PLASMID: PGEX-GP-1
KEYWDS      FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
KEYWDS      2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE
EXPDTA      X-RAY DIFFRACTION
AUTHOR      J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,I.SCHLEMMINGER,
AUTHOR      2 J.F.SEIBEL,C.J.SCHOFIELD
REVDAT      1   04-SEP-02 1H2M   0
JRNL        AUTH   J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,
JRNL        AUTH 2 I.SCHLEMMINGER,J.F.SEIBEL,C.J.SCHOFIELD
JRNL        TITL   FIH:HIF-FRAGMENT COMPLEXES
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK      2
REMARK      2 RESOLUTION. 2.5  ANGSTROMS.
REMARK      3
REMARK      3 REFINEMENT.
REMARK      3   PROGRAM      : REFMAC 5.0
REMARK      3   AUTHORS      : MURSHUDOV,VAGIN,DODSON
REMARK      3
REMARK      3   REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK      3
REMARK      3 DATA USED IN REFINEMENT.
REMARK      3   RESOLUTION RANGE HIGH (ANGSTROMS) :   2.50
REMARK      3   RESOLUTION RANGE LOW  (ANGSTROMS) :  18.00
REMARK      3   DATA CUTOFF          (SIGMA(F)) :  NONE
REMARK      3   COMPLETENESS FOR RANGE               (%) :  99.68
REMARK      3   NUMBER OF REFLECTIONS                  :  18404
REMARK      3
REMARK      3 FIT TO DATA USED IN REFINEMENT.

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REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE (WORKING + TEST SET) : 0.19432
REMARK 3 R VALUE (WORKING SET) : 0.19185
REMARK 3 FREE R VALUE : 0.22491
REMARK 3 FREE R VALUE TEST SET SIZE (%) : 7.6
REMARK 3 FREE R VALUE TEST SET COUNT : 1516
REMARK 3
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK 3 TOTAL NUMBER OF BINS USED : 20
REMARK 3 BIN RESOLUTION RANGE HIGH : 2.500
REMARK 3 BIN RESOLUTION RANGE LOW : 2.564
REMARK 3 REFLECTION IN BIN (WORKING SET) : 1267
REMARK 3 BIN R VALUE (WORKING SET) : 0.227
REMARK 3 BIN FREE R VALUE SET COUNT : 106
REMARK 3 BIN FREE R VALUE : 0.297
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 ALL ATOMS : 2979
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2) : NULL
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 35.778
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : -0.68
REMARK 3 B22 (A**2) : -0.68
REMARK 3 B33 (A**2) : 1.35
REMARK 3 B12 (A**2) : 0.00
REMARK 3 B13 (A**2) : 0.00
REMARK 3 B23 (A**2) : 0.00
REMARK 3
REMARK 3 ESTIMATED OVERALL COORDINATE ERROR.
REMARK 3 ESU BASED ON R VALUE (A) : 0.334
REMARK 3 ESU BASED ON FREE R VALUE (A) : 0.233
REMARK 3 ESU BASED ON MAXIMUM LIKELIHOOD (A) : 0.224
REMARK 3 ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2) : 9.825
REMARK 3
REMARK 3 CORRELATION COEFFICIENTS.
REMARK 3 CORRELATION COEFFICIENT FO-FC : 0.948
REMARK 3 CORRELATION COEFFICIENT FO-FC FREE : 0.935
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES COUNT RMS WEIGHT
REMARK 3 BOND LENGTHS REFINED ATOMS (A) : 2957 ; 0.017 ; 0.021
REMARK 3 BOND LENGTHS OTHERS (A) : 2546 ; 0.001 ; 0.020
REMARK 3 BOND ANGLES REFINED ATOMS (DEGREES) : 4022 ; 1.612 ; 1.948
REMARK 3 BOND ANGLES OTHERS (DEGREES) : 5944 ; 0.832 ; 3.000
REMARK 3 TORSION ANGLES, PERIOD 1 (DEGREES) : 350 ; 4.024 ; 3.000
REMARK 3 TORSION ANGLES, PERIOD 3 (DEGREES) : 512 ; 18.015 ; 15.000
REMARK 3 CHIRAL-CENTER RESTRAINTS (A**3) : 413 ; 0.097 ; 0.200
REMARK 3 GENERAL PLANES REFINED ATOMS (A) : 3315 ; 0.006 ; 0.020
REMARK 3 GENERAL PLANES OTHERS (A) : 602 ; 0.002 ; 0.020
REMARK 3 NON-BONDED CONTACTS REFINED ATOMS (A) : 731 ; 0.232 ; 0.300
REMARK 3 NON-BONDED CONTACTS OTHERS (A) : 2492 ; 0.214 ; 0.300
REMARK 3 H-BOND (X...Y) REFINED ATOMS (A) : 193 ; 0.173 ; 0.500
REMARK 3 H-BOND (X...Y) OTHERS (A) : 6 ; 0.126 ; 0.500
REMARK 3 POTENTIAL METAL-ION REFINED ATOMS (A) : 2 ; 0.054 ; 0.500
REMARK 3 SYMMETRY VDW REFINED ATOMS (A) : 15 ; 0.194 ; 0.300
REMARK 3 SYMMETRY VDW OTHERS (A) : 54 ; 0.255 ; 0.300
REMARK 3 SYMMETRY H-BOND REFINED ATOMS (A) : 7 ; 0.244 ; 0.500
REMARK 3 SYMMETRY H-BOND OTHERS (A) : 1 ; 0.053 ; 0.500
REMARK 3

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REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS.      COUNT    RMS    WEIGHT
REMARK 3 MAIN-CHAIN BOND REFINED ATOMS (A**2):    1767 ; 0.761 ; 1.500
REMARK 3 MAIN-CHAIN ANGLE REFINED ATOMS (A**2):    2846 ; 1.421 ; 2.000
REMARK 3 SIDE-CHAIN BOND REFINED ATOMS (A**2):    1190 ; 2.220 ; 3.000
REMARK 3 SIDE-CHAIN ANGLE REFINED ATOMS (A**2):    1176 ; 3.678 ; 4.500
REMARK 3
REMARK 3 NCS RESTRAINTS STATISTICS
REMARK 3 NUMBER OF NCS GROUPS : NULL
REMARK 3
REMARK 3 TLS DETAILS
REMARK 3 NUMBER OF TLS GROUPS : 1
REMARK 3
REMARK 3 TLS GROUP : 1
REMARK 3 NUMBER OF COMPONENTS GROUP : 2
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI
REMARK 3 RESIDUE RANGE : A 15 A 451
REMARK 3 RESIDUE RANGE : S 795 S 822
REMARK 3 ORIGIN FOR THE GROUP (A): 22.5990 26.9200 28.6340
REMARK 3 T TENSOR
REMARK 3 T11: 0.1903 T22: 0.0302
REMARK 3 T33: 0.0452 T12: -0.0025
REMARK 3 T13: -0.0536 T23: 0.0309
REMARK 3 L TENSOR
REMARK 3 L11: 0.7638 L22: 2.2674
REMARK 3 L33: 1.0629 L12: 0.7977
REMARK 3 L13: 0.4200 L23: 1.0769
REMARK 3 S TENSOR
REMARK 3 S11: 0.0306 S12: -0.1225 S13: -0.0490
REMARK 3 S21: 0.1656 S22: 0.0303 S23: 0.0478
REMARK 3 S31: 0.2046 S32: 0.0231 S33: -0.0609
REMARK 3
REMARK 3 BULK SOLVENT MODELLING.
REMARK 3 METHOD USED : BABINET MODEL WITH MASK
REMARK 3 PARAMETERS FOR MASK CALCULATION
REMARK 3 VDW PROBE RADIUS : 1.40
REMARK 3 ION PROBE RADIUS : 0.80
REMARK 3 SHRINKAGE RADIUS : 0.80
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS:
REMARK 3 HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
REMARK 4
REMARK 4 1H2M COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.
REMARK 100 THE EBI ID CODE IS EBI-11173.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION : 15-MAY-2002
REMARK 200 TEMPERATURE (KELVIN) : 100
REMARK 200 PH : 7.5
REMARK 200 NUMBER OF CRYSTALS USED : 1
REMARK 200
REMARK 200 SYNCHROTRON (Y/N) : Y
REMARK 200 RADIATION SOURCE : SRS BEAMLINE PX9.6
REMARK 200 BEAMLINE : PX9.6
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (A) : 0.87
REMARK 200 MONOCHROMATOR : NULL
REMARK 200 OPTICS : NULL

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REMARK 200  
REMARK 200 DETECTOR TYPE : ADSC QUANTUM 4  
REMARK 200 DETECTOR MANUFACTURER : ADSC  
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : MOSFLM  
REMARK 200 DATA SCALING SOFTWARE : SCALA  
REMARK 200  
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 20058  
REMARK 200 RESOLUTION RANGE HIGH (A) : 2.50  
REMARK 200 RESOLUTION RANGE LOW (A) : 87.71  
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NONE  
REMARK 200  
REMARK 200 OVERALL.  
REMARK 200 COMPLETENESS FOR RANGE (%) : 99.7  
REMARK 200 DATA REDUNDANCY : 6.5  
REMARK 200 R MERGE (I) : 0.050  
REMARK 200 R SYM (I) : NULL  
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 10.7  
REMARK 200  
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.  
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.50  
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A) : 2.64  
REMARK 200 COMPLETENESS FOR SHELL (%) : 97.9  
REMARK 200 DATA REDUNDANCY IN SHELL : 4.4  
REMARK 200 R MERGE FOR SHELL (I) : 0.289  
REMARK 200 R SYM FOR SHELL (I) : NULL  
REMARK 200 <I/SIGMA(I)> FOR SHELL : 2.6  
REMARK 200  
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH  
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT  
REMARK 200 SOFTWARE USED: NULL  
REMARK 200 STARTING MODEL: NULL  
REMARK 200  
REMARK 200 REMARK: NULL  
REMARK 280  
REMARK 280 CRYSTAL  
REMARK 280 SOLVENT CONTENT, VS (%): 63  
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS\*\*3/DA): 3.4  
REMARK 280  
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE,  
REMARK 280 4% PEG400, 0.1M HEPES PH7.5, 11MG/ML PROTEIN WITH  
REMARK 280 1MM FE(II), 2.5MM NOG AND 2.5MM PEPTIDE  
REMARK 290  
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY  
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2  
REMARK 290  
REMARK 290 SYMOP SYMMETRY  
REMARK 290 NNNMMM OPERATOR  
REMARK 290 1555 X, Y, Z  
REMARK 290 2555 -X, -Y, 1/2+Z  
REMARK 290 3555 1/2-Y, 1/2+X, 1/4+Z  
REMARK 290 4555 1/2+Y, 1/2-X, 3/4+Z  
REMARK 290 5555 1/2-X, 1/2+Y, 1/4-Z  
REMARK 290 6555 1/2+X, 1/2-Y, 3/4-Z  
REMARK 290 7555 Y, X, -Z  
REMARK 290 8555 -Y, -X, 1/2-Z  
REMARK 290  
REMARK 290 WHERE NNN -> OPERATOR NUMBER  
REMARK 290 MMM -> TRANSLATION VECTOR  
REMARK 290  
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS  
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM

REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY  
 REMARK 290 RELATED MOLECULES.

|            |        |   |           |           |           |           |
|------------|--------|---|-----------|-----------|-----------|-----------|
| REMARK 290 | SMTRY1 | 1 | 1.000000  | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 1 | 0.000000  | 1.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 1 | 0.000000  | 0.000000  | 1.000000  | 0.000000  |
| REMARK 290 | SMTRY1 | 2 | -1.000000 | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 2 | 0.000000  | -1.000000 | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 2 | 0.000000  | 0.000000  | 1.000000  | 74.13000  |
| REMARK 290 | SMTRY1 | 3 | 0.000000  | -1.000000 | 0.000000  | 43.12450  |
| REMARK 290 | SMTRY2 | 3 | 1.000000  | 0.000000  | 0.000000  | 43.12450  |
| REMARK 290 | SMTRY3 | 3 | 0.000000  | 0.000000  | 1.000000  | 37.06500  |
| REMARK 290 | SMTRY1 | 4 | 0.000000  | 1.000000  | 0.000000  | 43.12450  |
| REMARK 290 | SMTRY2 | 4 | -1.000000 | 0.000000  | 0.000000  | 43.12450  |
| REMARK 290 | SMTRY3 | 4 | 0.000000  | 0.000000  | 1.000000  | 111.19500 |
| REMARK 290 | SMTRY1 | 5 | -1.000000 | 0.000000  | 0.000000  | 43.12450  |
| REMARK 290 | SMTRY2 | 5 | 0.000000  | 1.000000  | 0.000000  | 43.12450  |
| REMARK 290 | SMTRY3 | 5 | 0.000000  | 0.000000  | -1.000000 | 37.06500  |
| REMARK 290 | SMTRY1 | 6 | 1.000000  | 0.000000  | 0.000000  | 43.12450  |
| REMARK 290 | SMTRY2 | 6 | 0.000000  | -1.000000 | 0.000000  | 43.12450  |
| REMARK 290 | SMTRY3 | 6 | 0.000000  | 0.000000  | -1.000000 | 111.19500 |
| REMARK 290 | SMTRY1 | 7 | 0.000000  | 1.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 7 | 1.000000  | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 7 | 0.000000  | 0.000000  | -1.000000 | 0.000000  |
| REMARK 290 | SMTRY1 | 8 | 0.000000  | -1.000000 | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY2 | 8 | -1.000000 | 0.000000  | 0.000000  | 0.000000  |
| REMARK 290 | SMTRY3 | 8 | 0.000000  | 0.000000  | -1.000000 | 74.13000  |

REMARK 290

REMARK 290 REMARK: NULL

REMARK 300

REMARK 300 BIOMOLECULE: 1

REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT  
 REMARK 300 WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR  
 REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).

REMARK 300

REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC

REMARK 300

REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.

REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S

REMARK 300 PRODUCES A TETRAMER.

REMARK 300

REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE

REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT

REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE

REMARK 300 HOMODIMER OF CHAIN A

REMARK 300

REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS

REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH

REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER

REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR

REMARK 300 THE CHAIN IN THE COMPLEX IS 2149.4 ANGSTROM\*\*2

REMARK 350

REMARK 350 GENERATING THE BIOMOLECULE

REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN

REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE

REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS

REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND

REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.

REMARK 350

REMARK 350 BIOMOLECULE: 1

REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S

REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 0.000000

|            |        |   |           |           |           |          |
|------------|--------|---|-----------|-----------|-----------|----------|
| REMARK 350 | BIOMT2 | 1 | 0.000000  | 1.000000  | 0.000000  | 0.000000 |
| REMARK 350 | BIOMT3 | 1 | 0.000000  | 0.000000  | 1.000000  | 0.000000 |
| REMARK 350 | BIOMT1 | 2 | 0.000000  | -1.000000 | 0.000000  | 86.24900 |
| REMARK 350 | BIOMT2 | 2 | -1.000000 | 0.000000  | 0.000000  | 86.24900 |
| REMARK 350 | BIOMT3 | 2 | 0.000000  | 0.000000  | -1.000000 | 74.13000 |

REMARK 465

REMARK 465 MISSING RESIDUES

REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE

REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN

REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)

REMARK 465

| M          | RES | C | SSSEQI |
|------------|-----|---|--------|
| REMARK 465 | MET | A | 1      |
| REMARK 465 | ALA | A | 2      |
| REMARK 465 | ALA | A | 3      |
| REMARK 465 | THR | A | 4      |
| REMARK 465 | ALA | A | 5      |
| REMARK 465 | ALA | A | 6      |
| REMARK 465 | GLU | A | 7      |
| REMARK 465 | ALA | A | 8      |
| REMARK 465 | VAL | A | 9      |
| REMARK 465 | ALA | A | 10     |
| REMARK 465 | SER | A | 11     |
| REMARK 465 | GLY | A | 12     |
| REMARK 465 | SER | A | 13     |
| REMARK 465 | GLY | A | 14     |
| REMARK 465 | LYS | A | 304    |
| REMARK 465 | ARG | A | 305    |
| REMARK 465 | ILE | A | 306    |
| REMARK 465 | PRO | S | 775    |
| REMARK 465 | SER | S | 776    |
| REMARK 465 | ASP | S | 777    |
| REMARK 465 | LEU | S | 778    |
| REMARK 465 | ALA | S | 779    |
| REMARK 465 | CYS | S | 780    |
| REMARK 465 | ARG | S | 781    |
| REMARK 465 | LEU | S | 782    |
| REMARK 465 | LEU | S | 783    |
| REMARK 465 | GLY | S | 784    |
| REMARK 465 | GLN | S | 785    |
| REMARK 465 | SER | S | 786    |
| REMARK 465 | MET | S | 787    |
| REMARK 465 | ASP | S | 788    |
| REMARK 465 | GLU | S | 789    |
| REMARK 465 | SER | S | 790    |
| REMARK 465 | GLY | S | 791    |
| REMARK 465 | LEU | S | 792    |
| REMARK 465 | PRO | S | 793    |
| REMARK 465 | GLN | S | 794    |
| REMARK 465 | GLN | S | 807    |
| REMARK 465 | GLY | S | 808    |
| REMARK 465 | SER | S | 809    |
| REMARK 465 | ARG | S | 810    |
| REMARK 465 | ASN | S | 811    |
| REMARK 465 | LEU | S | 812    |
| REMARK 465 | ASP | S | 823    |
| REMARK 465 | GLN | S | 824    |
| REMARK 465 | VAL | S | 825    |
| REMARK 465 | ASN | S | 826    |

REMARK 470

REMARK 470 MISSING ATOM



REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;  
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;  
REMARK 470 I=INSERTION CODE):

| M          | RES       | CSSEQI | ATOMS         |
|------------|-----------|--------|---------------|
| REMARK 470 | GLU A 15  | CG CD  | OE1 OE2       |
| REMARK 470 | GLU A 29  | CG CD  | OE1 OE2       |
| REMARK 470 | ASN A 87  | CG OD1 | ND2           |
| REMARK 470 | LYS A 106 | CD CE  | NZ            |
| REMARK 470 | LYS A 115 | CG CD  | CE NZ         |
| REMARK 470 | ARG A 117 | CG CD  | NE CZ NH1 NH2 |
| REMARK 470 | GLN A 133 | CG CD  | OE1 NE2       |
| REMARK 470 | GLN A 136 | CG CD  | OE1 NE2       |
| REMARK 470 | GLN A 137 | CG CD  | OE1 NE2       |
| REMARK 470 | ARG A 156 | CG CD  | NE CZ NH1 NH2 |
| REMARK 470 | LYS A 157 | CD CE  | NZ            |
| REMARK 470 | LYS A 311 | CG CD  | CE NZ         |

REMARK 500

REMARK 500 GEOMETRY AND STEREOCHEMISTRY

REMARK 500 SUBTOPIC: COVALENT BOND ANGLES

REMARK 500

REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES

REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE

REMARK 500 THAN 6\*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN

REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).

REMARK 500

REMARK 500 STANDARD TABLE:

REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)

REMARK 500

REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991

REMARK 500

| M          | RES       | CSSEQI | ATM1 | ATM2 | ATM3 |
|------------|-----------|--------|------|------|------|
| REMARK 500 | LEU A 227 | CA     | -    | CB   | -    |

REMARK 500 ANGL. DEV. = -11.0 DEGREES

REMARK 500

REMARK 500 REMARK: NULL

REMARK 500

REMARK 500 GEOMETRY AND STEREOCHEMISTRY

REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS

REMARK 500

REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES

REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE

REMARK 500 THAN 6\*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL

REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE

REMARK 500 NUMBER; I=INSERTION CODE).

REMARK 500

REMARK 500 STANDARD TABLE:

REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,1X,2(A4,A1,3X),12X,F5.3)

REMARK 500

REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991

REMARK 500

| M          | RES       | CSSEQI | ATM1 | RES       | CSSEQI | ATM2 | DEVIATION |
|------------|-----------|--------|------|-----------|--------|------|-----------|
| REMARK 500 | MET A 343 | SD     |      | MET A 343 | CE     |      | -0.209    |

REMARK 500

REMARK 500

REMARK 500 REMARK: NULL

REMARK 500

REMARK 500 GEOMETRY AND STEREOCHEMISTRY

REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT

REMARK 500

REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.

REMARK 500

| ATM1       | RES | C | SSEQI | ATM2 | RES | C | SSEQI | DISTANCE |
|------------|-----|---|-------|------|-----|---|-------|----------|
| REMARK 500 |     |   |       |      |     |   |       |          |

REMARK 500

REMARK 500 O ALA A 300 OH TYR S 798 2.09  
REMARK 525  
REMARK 525 SOLVENT  
REMARK 525  
REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO  
REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY  
REMARK 525 ASSOCIATED WITH:  
REMARK 525 PROTEIN CHAIN SOLVENT CHAIN  
REMARK 525 A Z  
REMARK 525 S H  
REMARK 600  
REMARK 600 HETEROGEN  
REMARK 600  
REMARK 600 FOR METAL ATOM ZN ZN A1350 THE COORDINATION ANGLES ARE:  
REMARK 600 1 HIS 199A NE2 103.4  
REMARK 600 2 ASP 201A OD2 84.2 88.5  
REMARK 600 3 HIS 279A NE2 169.0 87.2 99.0  
REMARK 600 4 OGA 1351A O2 86.3 169.1 97.3 82.8  
REMARK 600 5 OGA 1351A O2' 1 2 3 4  
REMARK 600  
REMARK 700  
REMARK 700 SHEET  
REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN  
REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,  
REMARK 700 TWO SHEETS ARE DEFINED.  
REMARK 800  
REMARK 800 SITE  
REMARK 800 SITE\_IDENTIFIER: ZNA  
REMARK 800 SITE\_DESCRIPTION: ZN BINDING SITE FOR CHAIN A  
REMARK 800  
REMARK 800 SITE\_IDENTIFIER: OGA  
REMARK 800 SITE\_DESCRIPTION: OGA BINDING SITE FOR CHAIN A  
REMARK 800  
REMARK 800 SITE\_IDENTIFIER: SA1  
REMARK 800 SITE\_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A  
REMARK 800  
REMARK 800 SITE\_IDENTIFIER: SA2  
REMARK 800 SITE\_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A  
REMARK 900  
REMARK 900 RELATED ENTRIES  
REMARK 900 RELATED ID: 1D7G RELATED DB: PDB  
REMARK 900 A MODEL FOR THE COMPLEX BETWEEN THE  
REMARK 900 HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS  
REMARK 900 CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE  
REMARK 900 RELATED ID: 1H2K RELATED DB: PDB  
REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX  
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE  
REMARK 900 RELATED ID: 1H2L RELATED DB: PDB  
REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX  
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE  
REMARK 900 RELATED ID: 1H2N RELATED DB: PDB  
REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX  
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE  
REMARK 900 RELATED ID: 1L8C RELATED DB: PDB  
REMARK 900 STRUCTURAL BASIS FOR HIF-1ALPHA/CBP  
REMARK 900 RECOGNITION IN THECELLULAR HYPOXIC RESPONSE  
REMARK 900 RELATED ID: 1LM8 RELATED DB: PDB  
REMARK 900 STRUCTURE OF A HIF-1A-PVHL-ELONGINB-  
REMARK 900 ELONGINC COMPLEX  
REMARK 900 RELATED ID: 1LQB RELATED DB: PDB  
REMARK 900 CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1

REMARK 900 ELONGIN-B COMPLEX

|        |                     |                   |   |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
|--------|---------------------|-------------------|---|-------|--------|------------|-----|-----|--|--|--|--|--|--|--|--|--|
| REMARK | 900                 | ELONGIN-B COMPLEX |   |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| DBREF  | 1H2M A              | 1                 | 349   | SWS   | Q969Q7 | Q969Q7     | 1   | 349 |  |  |  |  |  |  |  |  |  |
| DBREF  | 1H2M S              | 775               | 826   | SWS   | Q16665 | HIFA_HUMAN | 775 | 826 |  |  |  |  |  |  |  |  |  |
| SEQRES | 1 A                 | 349               | MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 2 A                 | 349               | GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 3 A                 | 349               | TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 4 A                 | 349               | ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 5 A                 | 349               | GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 6 A                 | 349               | ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 7 A                 | 349               | GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 8 A                 | 349               | VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 9 A                 | 349               | GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 10 A                | 349               | SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 11 A                | 349               | LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 12 A                | 349               | LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 13 A                | 349               | LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 14 A                | 349               | ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 15 A                | 349               | THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 16 A                | 349               | THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 17 A                | 349               | GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 18 A                | 349               | ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 19 A                | 349               | PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 20 A                | 349               | ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 21 A                | 349               | TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 22 A                | 349               | PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 23 A                | 349               | GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 24 A                | 349               | ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 25 A                | 349               | HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 26 A                | 349               | LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 27 A                | 349               | LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN         |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 1 S                 | 52                | PRO SER ASP LEU ALA CYS ARG LEU LEU GLY GLN SER MET |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 2 S                 | 52                | ASP GLU SER GLY LEU PRO GLN LEU THR SER TYR ASP CYS |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 3 S                 | 52                | GLU VAL ASN ALA PRO ILE GLN GLY SER ARG ASN LEU LEU |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| SEQRES | 4 S                 | 52                | GLN GLY GLU GLU LEU LEU ARG ALA LEU ASP GLN VAL ASN |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| HET    | ZN                  | A1350             | 1   |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| HET    | OGA                 | A1351             | 10  |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| HET    | SO4                 | A1352             | 5   |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| HET    | SO4                 | A1353             | 5   |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| HETNAM | ZN ZINC ION         |                   |   |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| HETNAM | OGA N-OXALYLGLYCINE |                   |   |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| HETNAM | SO4 SULFATE ION     |                   |   |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| FORMUL | 3                   | ZN                | ZN1 2+  |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| FORMUL | 4                   | OGA               | C4 H5 N1 O5   |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| FORMUL | 5                   | SO4               | 2(O4 S1 2-)   |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| FORMUL | 6                   | HOH               | *99(H2 O1)  |       |        |            |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 1                   | 1 ASP A           | 28  | LEU A | 32     | 5          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 2                   | 2 ASP A           | 49  | ASN A | 58     | 1          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 3                   | 3 VAL A           | 70  | TRP A | 76     | 5          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 4                   | 4 ASP A           | 77  | ILE A | 85     | 1          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 5                   | 5 ASP A           | 104   | GLN A | 112    | 5          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 6                   | 6 LYS A           | 124   | ARG A | 138    | 1          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 7                   | 7 GLY A           | 155   | GLY A | 164    | 1          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 8                   | 8 ASN A           | 166   | ARG A | 177    | 1          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 9                   | 9 PRO A           | 220   | ASP A | 222    | 5          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 10                  | 10 GLN A          | 223   | TYR A | 228    | 1          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 11                  | 11 PHE A          | 252   | VAL A | 258    | 5          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 12                  | 12 LYS A          | 311   | GLY A | 331    | 1          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 13                  | 13 ASN A          | 332   | GLN A | 334    | 5          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 14                  | 14 GLU A          | 335   | LYS A | 345    | 1          |     |     |  |  |  |  |  |  |  |  |  |
| HELIX  | 15                  | 15 GLN S          | 814   | LEU S | 822    | 1          |     |     |  |  |  |  |  |  |  |  |  |

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|      |    |     |     |   |    |        |        |        |      |       |   |
|------|----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 21 | CZ  | ARG | A | 17 | 11.401 | 24.776 | 12.744 | 1.00 | 84.27 | C |
| ATOM | 22 | NH1 | ARG | A | 17 | 11.980 | 25.968 | 12.584 | 1.00 | 83.33 | N |
| ATOM | 23 | NH2 | ARG | A | 17 | 11.311 | 24.268 | 13.967 | 1.00 | 85.10 | N |
| ATOM | 24 | N   | GLU | A | 18 | 5.796  | 24.209 | 8.421  | 1.00 | 74.01 | N |
| ATOM | 25 | CA  | GLU | A | 18 | 4.692  | 23.274 | 8.319  | 1.00 | 72.99 | C |
| ATOM | 26 | C   | GLU | A | 18 | 5.193  | 21.855 | 8.607  | 1.00 | 71.43 | C |
| ATOM | 27 | O   | GLU | A | 18 | 6.210  | 21.421 | 8.061  | 1.00 | 70.71 | O |
| ATOM | 28 | CB  | GLU | A | 18 | 4.033  | 23.352 | 6.938  | 1.00 | 73.29 | C |
| ATOM | 29 | CG  | GLU | A | 18 | 3.333  | 24.677 | 6.659  | 1.00 | 73.91 | C |
| ATOM | 30 | CD  | GLU | A | 18 | 1.949  | 24.794 | 7.283  | 1.00 | 74.30 | C |
| ATOM | 31 | OE1 | GLU | A | 18 | 1.355  | 23.776 | 7.692  | 1.00 | 74.07 | O |
| ATOM | 32 | OE2 | GLU | A | 18 | 1.444  | 25.929 | 7.356  | 1.00 | 75.76 | O |
| ATOM | 33 | N   | GLU | A | 19 | 4.482  | 21.157 | 9.491  | 1.00 | 69.89 | N |
| ATOM | 34 | CA  | GLU | A | 19 | 4.786  | 19.764 | 9.818  | 1.00 | 68.89 | C |
| ATOM | 35 | C   | GLU | A | 19 | 4.393  | 18.854 | 8.661  | 1.00 | 66.65 | C |
| ATOM | 36 | O   | GLU | A | 19 | 3.324  | 19.011 | 8.065  | 1.00 | 65.92 | O |
| ATOM | 37 | CB  | GLU | A | 19 | 4.058  | 19.311 | 11.096 | 1.00 | 69.41 | C |
| ATOM | 38 | CG  | GLU | A | 19 | 4.544  | 19.996 | 12.370 | 1.00 | 72.06 | C |
| ATOM | 39 | CD  | GLU | A | 19 | 4.308  | 19.194 | 13.657 | 1.00 | 76.41 | C |
| ATOM | 40 | OE1 | GLU | A | 19 | 3.855  | 18.016 | 13.609 | 1.00 | 78.21 | O |
| ATOM | 41 | OE2 | GLU | A | 19 | 4.590  | 19.758 | 14.746 | 1.00 | 79.64 | O |
| ATOM | 42 | N   | ALA | A | 20 | 5.283  | 17.919 | 8.349  | 1.00 | 64.54 | N |
| ATOM | 43 | CA  | ALA | A | 20 | 5.067  | 16.921 | 7.303  | 1.00 | 63.03 | C |
| ATOM | 44 | C   | ALA | A | 20 | 3.735  | 16.225 | 7.449  | 1.00 | 61.23 | C |
| ATOM | 45 | O   | ALA | A | 20 | 3.303  | 15.903 | 8.556  | 1.00 | 60.61 | O |
| ATOM | 46 | CB  | ALA | A | 20 | 6.177  | 15.889 | 7.312  | 1.00 | 62.82 | C |
| ATOM | 47 | N   | GLY | A | 21 | 3.087  | 16.002 | 6.316  | 1.00 | 59.29 | N |
| ATOM | 48 | CA  | GLY | A | 21 | 1.833  | 15.289 | 6.304  | 1.00 | 58.26 | C |
| ATOM | 49 | C   | GLY | A | 21 | 0.651  | 16.200 | 6.530  | 1.00 | 57.44 | C |
| ATOM | 50 | O   | GLY | A | 21 | -0.416 | 15.739 | 6.873  | 1.00 | 56.42 | O |
| ATOM | 51 | N   | ALA | A | 22 | 0.858  | 17.500 | 6.341  | 1.00 | 57.28 | N |
| ATOM | 52 | CA  | ALA | A | 22 | -0.182 | 18.509 | 6.492  | 1.00 | 56.92 | C |
| ATOM | 53 | C   | ALA | A | 22 | -0.737 | 18.544 | 7.909  | 1.00 | 56.53 | C |
| ATOM | 54 | O   | ALA | A | 22 | -1.926 | 18.737 | 8.108  | 1.00 | 56.32 | O |
| ATOM | 55 | CB  | ALA | A | 22 | -1.285 | 18.277 | 5.488  | 1.00 | 57.10 | C |
| ATOM | 56 | N   | LEU | A | 23 | 0.133  | 18.369 | 8.898  | 1.00 | 56.25 | N |
| ATOM | 57 | CA  | LEU | A | 23 | -0.306 | 18.397 | 10.289 | 1.00 | 56.07 | C |
| ATOM | 58 | C   | LEU | A | 23 | -0.385 | 19.811 | 10.827 | 1.00 | 55.03 | C |
| ATOM | 59 | O   | LEU | A | 23 | -0.638 | 20.037 | 11.998 | 1.00 | 54.89 | O |
| ATOM | 60 | CB  | LEU | A | 23 | 0.583  | 17.519 | 11.149 | 1.00 | 56.05 | C |
| ATOM | 61 | CG  | LEU | A | 23 | 0.445  | 16.067 | 10.678 | 1.00 | 58.06 | C |
| ATOM | 62 | CD1 | LEU | A | 23 | 1.307  | 15.080 | 11.478 | 1.00 | 59.22 | C |
| ATOM | 63 | CD2 | LEU | A | 23 | -1.030 | 15.653 | 10.735 | 1.00 | 59.53 | C |
| ATOM | 64 | N   | GLY | A | 24 | -0.202 | 20.768 | 9.941  | 1.00 | 54.17 | N |
| ATOM | 65 | CA  | GLY | A | 24 | -0.337 | 22.151 | 10.305 | 1.00 | 53.43 | C |
| ATOM | 66 | C   | GLY | A | 24 | 0.932  | 22.758 | 10.834 | 1.00 | 52.71 | C |
| ATOM | 67 | O   | GLY | A | 24 | 2.025  | 22.189 | 10.807 | 1.00 | 52.28 | O |
| ATOM | 68 | N   | PRO | A | 25 | 0.775  | 23.965 | 11.324 | 1.00 | 51.60 | N |
| ATOM | 69 | CA  | PRO | A | 25 | 1.908  | 24.695 | 11.858 | 1.00 | 50.67 | C |
| ATOM | 70 | C   | PRO | A | 25 | 2.310  | 24.047 | 13.168 | 1.00 | 49.52 | C |
| ATOM | 71 | O   | PRO | A | 25 | 1.481  | 23.648 | 13.982 | 1.00 | 47.61 | O |
| ATOM | 72 | CB  | PRO | A | 25 | 1.366  | 26.110 | 12.065 | 1.00 | 50.61 | C |
| ATOM | 73 | CG  | PRO | A | 25 | -0.109 | 26.034 | 11.931 | 1.00 | 50.61 | C |
| ATOM | 74 | CD  | PRO | A | 25 | -0.493 | 24.689 | 11.463 | 1.00 | 51.58 | C |
| ATOM | 75 | N   | ALA | A | 26 | 3.616  | 23.922 | 13.321 | 1.00 | 49.47 | N |
| ATOM | 76 | CA  | ALA | A | 26 | 4.218  | 23.390 | 14.526 | 1.00 | 49.29 | C |
| ATOM | 77 | C   | ALA | A | 26 | 3.894  | 24.266 | 15.759 | 1.00 | 47.94 | C |
| ATOM | 78 | O   | ALA | A | 26 | 3.646  | 23.735 | 16.836 | 1.00 | 48.27 | O |
| ATOM | 79 | CB  | ALA | A | 26 | 5.712  | 23.288 | 14.328 | 1.00 | 49.68 | C |
| ATOM | 80 | N   | TRP | A | 27 | 3.864  | 25.581 | 15.592 | 1.00 | 45.91 | N |
| ATOM | 81 | CA  | TRP | A | 27 | 3.494  | 26.487 | 16.683 | 1.00 | 45.16 | C |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 82  | C   | TRP | A | 27 | 3.003  | 27.818 | 16.107 | 1.00 | 44.47 | C |
| ATOM | 83  | O   | TRP | A | 27 | 2.985  | 27.981 | 14.901 | 1.00 | 44.30 | O |
| ATOM | 84  | CB  | TRP | A | 27 | 4.719  | 26.727 | 17.568 | 1.00 | 44.91 | C |
| ATOM | 85  | CG  | TRP | A | 27 | 5.916  | 26.910 | 16.737 | 1.00 | 42.67 | C |
| ATOM | 86  | CD1 | TRP | A | 27 | 6.702  | 25.934 | 16.197 | 1.00 | 43.38 | C |
| ATOM | 87  | CD2 | TRP | A | 27 | 6.411  | 28.129 | 16.255 | 1.00 | 38.70 | C |
| ATOM | 88  | NE1 | TRP | A | 27 | 7.690  | 26.494 | 15.425 | 1.00 | 41.56 | N |
| ATOM | 89  | CE2 | TRP | A | 27 | 7.532  | 27.847 | 15.452 | 1.00 | 39.59 | C |
| ATOM | 90  | CE3 | TRP | A | 27 | 6.039  | 29.442 | 16.431 | 1.00 | 38.28 | C |
| ATOM | 91  | CZ2 | TRP | A | 27 | 8.284  | 28.827 | 14.861 | 1.00 | 39.74 | C |
| ATOM | 92  | CZ3 | TRP | A | 27 | 6.781  | 30.409 | 15.849 | 1.00 | 39.48 | C |
| ATOM | 93  | CH2 | TRP | A | 27 | 7.884  | 30.104 | 15.057 | 1.00 | 40.17 | C |
| ATOM | 94  | N   | ASP | A | 28 | 2.580  | 28.760 | 16.941 | 1.00 | 43.91 | N |
| ATOM | 95  | CA  | ASP | A | 28 | 2.230  | 30.079 | 16.417 | 1.00 | 43.87 | C |
| ATOM | 96  | C   | ASP | A | 28 | 2.750  | 31.161 | 17.305 | 1.00 | 42.33 | C |
| ATOM | 97  | O   | ASP | A | 28 | 3.191  | 30.901 | 18.409 | 1.00 | 42.11 | O |
| ATOM | 98  | CB  | ASP | A | 28 | 0.722  | 30.251 | 16.199 | 1.00 | 44.82 | C |
| ATOM | 99  | CG  | ASP | A | 28 | -0.052 | 30.162 | 17.462 | 1.00 | 47.87 | C |
| ATOM | 100 | OD1 | ASP | A | 28 | -0.240 | 31.236 | 18.108 | 1.00 | 50.91 | O |
| ATOM | 101 | OD2 | ASP | A | 28 | -0.501 | 29.054 | 17.877 | 1.00 | 49.06 | O |
| ATOM | 102 | N   | GLU | A | 29 | 2.713  | 32.385 | 16.790 | 1.00 | 41.29 | N |
| ATOM | 103 | CA  | GLU | A | 29 | 3.208  | 33.586 | 17.499 | 1.00 | 39.69 | C |
| ATOM | 104 | C   | GLU | A | 29 | 2.685  | 33.711 | 18.917 | 1.00 | 37.94 | C |
| ATOM | 105 | O   | GLU | A | 29 | 3.415  | 34.069 | 19.801 | 1.00 | 37.26 | O |
| ATOM | 106 | CB  | GLU | A | 29 | 2.840  | 34.812 | 16.735 | 1.00 | 39.59 | C |
| ATOM | 107 | N   | SER | A | 30 | 1.427  | 33.371 | 19.135 | 1.00 | 36.78 | N |
| ATOM | 108 | CA  | SER | A | 30 | 0.810  | 33.558 | 20.443 | 1.00 | 36.13 | C |
| ATOM | 109 | C   | SER | A | 30 | 1.501  | 32.756 | 21.517 | 1.00 | 35.30 | C |
| ATOM | 110 | O   | SER | A | 30 | 1.252  | 32.968 | 22.678 | 1.00 | 35.21 | O |
| ATOM | 111 | CB  | SER | A | 30 | -0.686 | 33.180 | 20.406 | 1.00 | 35.84 | C |
| ATOM | 112 | OG  | SER | A | 30 | -0.901 | 31.762 | 20.450 | 1.00 | 36.93 | O |
| ATOM | 113 | N   | GLN | A | 31 | 2.326  | 31.795 | 21.116 | 1.00 | 35.24 | N |
| ATOM | 114 | CA  | GLN | A | 31 | 3.021  | 30.918 | 22.060 | 1.00 | 34.89 | C |
| ATOM | 115 | C   | GLN | A | 31 | 4.366  | 31.506 | 22.487 | 1.00 | 34.60 | C |
| ATOM | 116 | O   | GLN | A | 31 | 5.010  | 30.969 | 23.365 | 1.00 | 34.18 | O |
| ATOM | 117 | CB  | GLN | A | 31 | 3.224  | 29.513 | 21.473 | 1.00 | 34.65 | C |
| ATOM | 118 | CG  | GLN | A | 31 | 1.969  | 28.649 | 21.402 | 1.00 | 34.74 | C |
| ATOM | 119 | CD  | GLN | A | 31 | 2.212  | 27.322 | 20.707 | 1.00 | 33.47 | C |
| ATOM | 120 | OE1 | GLN | A | 31 | 2.215  | 27.249 | 19.476 | 1.00 | 32.57 | O |
| ATOM | 121 | NE2 | GLN | A | 31 | 2.442  | 26.278 | 21.492 | 1.00 | 32.95 | N |
| ATOM | 122 | N   | LEU | A | 32 | 4.753  | 32.632 | 21.895 | 1.00 | 34.85 | N |
| ATOM | 123 | CA  | LEU | A | 32 | 6.016  | 33.293 | 22.212 | 1.00 | 35.01 | C |
| ATOM | 124 | C   | LEU | A | 32 | 5.798  | 34.391 | 23.223 | 1.00 | 34.91 | C |
| ATOM | 125 | O   | LEU | A | 32 | 4.834  | 35.134 | 23.125 | 1.00 | 35.83 | O |
| ATOM | 126 | CB  | LEU | A | 32 | 6.631  | 33.885 | 20.945 | 1.00 | 34.96 | C |
| ATOM | 127 | CG  | LEU | A | 32 | 6.995  | 32.860 | 19.849 | 1.00 | 36.03 | C |
| ATOM | 128 | CD1 | LEU | A | 32 | 7.691  | 33.525 | 18.701 | 1.00 | 36.15 | C |
| ATOM | 129 | CD2 | LEU | A | 32 | 7.855  | 31.780 | 20.377 | 1.00 | 35.18 | C |
| ATOM | 130 | N   | ARG | A | 33 | 6.675  | 34.500 | 24.209 | 1.00 | 34.49 | N |
| ATOM | 131 | CA  | ARG | A | 33 | 6.564  | 35.591 | 25.170 | 1.00 | 34.33 | C |
| ATOM | 132 | C   | ARG | A | 33 | 7.005  | 36.867 | 24.460 | 1.00 | 34.37 | C |
| ATOM | 133 | O   | ARG | A | 33 | 7.733  | 36.815 | 23.498 | 1.00 | 34.87 | O |
| ATOM | 134 | CB  | ARG | A | 33 | 7.442  | 35.338 | 26.394 | 1.00 | 34.16 | C |
| ATOM | 135 | CG  | ARG | A | 33 | 7.056  | 34.124 | 27.212 | 1.00 | 32.83 | C |
| ATOM | 136 | CD  | ARG | A | 33 | 7.951  | 33.894 | 28.428 | 1.00 | 33.34 | C |
| ATOM | 137 | NE  | ARG | A | 33 | 7.413  | 32.820 | 29.252 | 1.00 | 34.91 | N |
| ATOM | 138 | CZ  | ARG | A | 33 | 6.445  | 32.963 | 30.137 | 1.00 | 36.53 | C |
| ATOM | 139 | NH1 | ARG | A | 33 | 5.900  | 34.144 | 30.382 | 1.00 | 34.89 | N |
| ATOM | 140 | NH2 | ARG | A | 33 | 6.027  | 31.905 | 30.795 | 1.00 | 39.39 | N |
| ATOM | 141 | N   | SER | A | 34 | 6.608  | 38.022 | 24.947 | 1.00 | 34.36 | N |
| ATOM | 142 | CA  | SER | A | 34 | 6.944  | 39.247 | 24.244 | 1.00 | 34.69 | C |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 143 | C   | SER | A | 34 | 8.002  | 40.055 | 24.987 | 1.00 | 33.26 | C |
| ATOM | 144 | O   | SER | A | 34 | 7.958  | 40.142 | 26.200 | 1.00 | 33.50 | O |
| ATOM | 145 | CB  | SER | A | 34 | 5.698  | 40.096 | 24.143 | 1.00 | 35.23 | C |
| ATOM | 146 | OG  | SER | A | 34 | 5.586  | 40.744 | 25.393 | 1.00 | 39.99 | O |
| ATOM | 147 | N   | TYR | A | 35 | 8.911  | 40.682 | 24.252 | 1.00 | 32.38 | N |
| ATOM | 148 | CA  | TYR | A | 35 | 10.080 | 41.329 | 24.843 | 1.00 | 32.03 | C |
| ATOM | 149 | C   | TYR | A | 35 | 10.339 | 42.675 | 24.193 | 1.00 | 32.52 | C |
| ATOM | 150 | O   | TYR | A | 35 | 9.763  | 42.979 | 23.172 | 1.00 | 32.78 | O |
| ATOM | 151 | CB  | TYR | A | 35 | 11.290 | 40.422 | 24.686 | 1.00 | 31.20 | C |
| ATOM | 152 | CG  | TYR | A | 35 | 11.139 | 39.161 | 25.482 | 1.00 | 30.69 | C |
| ATOM | 153 | CD1 | TYR | A | 35 | 10.935 | 39.215 | 26.853 | 1.00 | 30.40 | C |
| ATOM | 154 | CD2 | TYR | A | 35 | 11.186 | 37.915 | 24.875 | 1.00 | 30.34 | C |
| ATOM | 155 | CE1 | TYR | A | 35 | 10.804 | 38.054 | 27.609 | 1.00 | 31.74 | C |
| ATOM | 156 | CE2 | TYR | A | 35 | 11.050 | 36.741 | 25.617 | 1.00 | 32.05 | C |
| ATOM | 157 | CZ  | TYR | A | 35 | 10.858 | 36.812 | 26.991 | 1.00 | 31.98 | C |
| ATOM | 158 | OH  | TYR | A | 35 | 10.687 | 35.658 | 27.742 | 1.00 | 30.13 | O |
| ATOM | 159 | N   | SER | A | 36 | 11.240 | 43.463 | 24.761 | 1.00 | 33.06 | N |
| ATOM | 160 | CA  | SER | A | 36 | 11.469 | 44.838 | 24.289 | 1.00 | 32.95 | C |
| ATOM | 161 | C   | SER | A | 36 | 12.469 | 44.977 | 23.159 | 1.00 | 32.65 | C |
| ATOM | 162 | O   | SER | A | 36 | 12.705 | 46.084 | 22.674 | 1.00 | 33.04 | O |
| ATOM | 163 | CB  | SER | A | 36 | 11.979 | 45.698 | 25.438 | 1.00 | 32.92 | C |
| ATOM | 164 | OG  | SER | A | 36 | 13.272 | 45.325 | 25.844 | 1.00 | 33.05 | O |
| ATOM | 165 | N   | PHE | A | 37 | 13.041 | 43.880 | 22.711 | 1.00 | 31.44 | N |
| ATOM | 166 | CA  | PHE | A | 37 | 14.100 | 43.988 | 21.740 | 1.00 | 31.55 | C |
| ATOM | 167 | C   | PHE | A | 37 | 13.784 | 43.269 | 20.444 | 1.00 | 31.69 | C |
| ATOM | 168 | O   | PHE | A | 37 | 13.020 | 42.326 | 20.386 | 1.00 | 32.65 | O |
| ATOM | 169 | CB  | PHE | A | 37 | 15.421 | 43.431 | 22.339 | 1.00 | 30.68 | C |
| ATOM | 170 | CG  | PHE | A | 37 | 15.275 | 42.054 | 22.890 | 1.00 | 30.10 | C |
| ATOM | 171 | CD1 | PHE | A | 37 | 15.329 | 40.967 | 22.060 | 1.00 | 28.43 | C |
| ATOM | 172 | CD2 | PHE | A | 37 | 15.022 | 41.852 | 24.231 | 1.00 | 29.43 | C |
| ATOM | 173 | CE1 | PHE | A | 37 | 15.168 | 39.679 | 22.564 | 1.00 | 31.59 | C |
| ATOM | 174 | CE2 | PHE | A | 37 | 14.852 | 40.580 | 24.733 | 1.00 | 30.52 | C |
| ATOM | 175 | CZ  | PHE | A | 37 | 14.927 | 39.495 | 23.915 | 1.00 | 31.81 | C |
| ATOM | 176 | N   | PRO | A | 38 | 14.403 | 43.721 | 19.384 | 1.00 | 31.70 | N |
| ATOM | 177 | CA  | PRO | A | 38 | 14.268 | 43.036 | 18.106 | 1.00 | 31.23 | C |
| ATOM | 178 | C   | PRO | A | 38 | 15.231 | 41.895 | 17.984 | 1.00 | 31.71 | C |
| ATOM | 179 | O   | PRO | A | 38 | 16.205 | 41.880 | 18.743 | 1.00 | 31.59 | O |
| ATOM | 180 | CB  | PRO | A | 38 | 14.652 | 44.118 | 17.117 | 1.00 | 31.44 | C |
| ATOM | 181 | CG  | PRO | A | 38 | 15.636 | 45.005 | 17.922 | 1.00 | 32.43 | C |
| ATOM | 182 | CD  | PRO | A | 38 | 15.186 | 44.973 | 19.320 | 1.00 | 30.26 | C |
| ATOM | 183 | N   | THR | A | 39 | 14.996 | 41.008 | 17.003 | 1.00 | 31.90 | N |
| ATOM | 184 | CA  | THR | A | 39 | 15.868 | 39.891 | 16.702 | 1.00 | 32.00 | C |
| ATOM | 185 | C   | THR | A | 39 | 15.865 | 39.606 | 15.203 | 1.00 | 32.89 | C |
| ATOM | 186 | O   | THR | A | 39 | 14.998 | 40.048 | 14.476 | 1.00 | 32.28 | O |
| ATOM | 187 | CB  | THR | A | 39 | 15.370 | 38.647 | 17.377 | 1.00 | 32.26 | C |
| ATOM | 188 | OG1 | THR | A | 39 | 14.024 | 38.389 | 16.949 | 1.00 | 30.59 | O |
| ATOM | 189 | CG2 | THR | A | 39 | 15.235 | 38.832 | 18.905 | 1.00 | 32.99 | C |
| ATOM | 190 | N   | ARG | A | 40 | 16.855 | 38.844 | 14.770 | 1.00 | 33.28 | N |
| ATOM | 191 | CA  | ARG | A | 40 | 16.980 | 38.372 | 13.421 | 1.00 | 34.30 | C |
| ATOM | 192 | C   | ARG | A | 40 | 17.023 | 36.853 | 13.562 | 1.00 | 33.77 | C |
| ATOM | 193 | O   | ARG | A | 40 | 17.288 | 36.324 | 14.614 | 1.00 | 34.68 | O |
| ATOM | 194 | CB  | ARG | A | 40 | 18.267 | 38.847 | 12.795 | 1.00 | 34.73 | C |
| ATOM | 195 | CG  | ARG | A | 40 | 18.273 | 40.306 | 12.451 | 1.00 | 41.24 | C |
| ATOM | 196 | CD  | ARG | A | 40 | 16.909 | 40.799 | 12.022 | 1.00 | 48.38 | C |
| ATOM | 197 | NE  | ARG | A | 40 | 16.728 | 41.025 | 10.597 | 1.00 | 51.83 | N |
| ATOM | 198 | CZ  | ARG | A | 40 | 15.553 | 41.291 | 10.092 | 1.00 | 56.70 | C |
| ATOM | 199 | NH1 | ARG | A | 40 | 14.501 | 41.300 | 10.908 | 1.00 | 57.84 | N |
| ATOM | 200 | NH2 | ARG | A | 40 | 15.415 | 41.549 | 8.795  | 1.00 | 60.30 | N |
| ATOM | 201 | N   | PRO | A | 41 | 16.663 | 36.147 | 12.533 | 1.00 | 33.50 | N |
| ATOM | 202 | CA  | PRO | A | 41 | 16.646 | 34.681 | 12.569 | 1.00 | 33.48 | C |
| ATOM | 203 | C   | PRO | A | 41 | 18.002 | 34.010 | 12.475 | 1.00 | 32.72 | C |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 204 | O   | PRO | A | 41 | 18.907 | 34.475 | 11.801 | 1.00 | 34.64 | O |
| ATOM | 205 | CB  | PRO | A | 41 | 15.800 | 34.299 | 11.340 | 1.00 | 33.22 | C |
| ATOM | 206 | CG  | PRO | A | 41 | 15.409 | 35.563 | 10.675 | 1.00 | 33.55 | C |
| ATOM | 207 | CD  | PRO | A | 41 | 16.038 | 36.717 | 11.343 | 1.00 | 32.95 | C |
| ATOM | 208 | N   | ILE | A | 42 | 18.154 | 32.925 | 13.192 | 1.00 | 30.97 | N |
| ATOM | 209 | CA  | ILE | A | 42 | 19.337 | 32.144 | 13.049 | 1.00 | 29.87 | C |
| ATOM | 210 | C   | ILE | A | 42 | 19.077 | 31.289 | 11.814 | 1.00 | 30.07 | C |
| ATOM | 211 | O   | ILE | A | 42 | 17.946 | 30.857 | 11.587 | 1.00 | 30.17 | O |
| ATOM | 212 | CB  | ILE | A | 42 | 19.477 | 31.306 | 14.273 | 1.00 | 29.85 | C |
| ATOM | 213 | CG1 | ILE | A | 42 | 19.721 | 32.215 | 15.478 | 1.00 | 27.79 | C |
| ATOM | 214 | CG2 | ILE | A | 42 | 20.582 | 30.264 | 14.105 | 1.00 | 30.60 | C |
| ATOM | 215 | CD1 | ILE | A | 42 | 19.565 | 31.503 | 16.788 | 1.00 | 25.35 | C |
| ATOM | 216 | N   | PRO | A | 43 | 20.085 | 31.075 | 10.985 | 1.00 | 29.34 | N |
| ATOM | 217 | CA  | PRO | A | 43 | 19.922 | 30.219 | 9.823  | 1.00 | 29.60 | C |
| ATOM | 218 | C   | PRO | A | 43 | 19.623 | 28.751 | 10.176 | 1.00 | 30.65 | C |
| ATOM | 219 | O   | PRO | A | 43 | 20.207 | 28.265 | 11.160 | 1.00 | 31.73 | O |
| ATOM | 220 | CB  | PRO | A | 43 | 21.288 | 30.310 | 9.139  | 1.00 | 30.00 | C |
| ATOM | 221 | CG  | PRO | A | 43 | 21.933 | 31.491 | 9.665  | 1.00 | 28.87 | C |
| ATOM | 222 | CD  | PRO | A | 43 | 21.420 | 31.676 | 11.047 | 1.00 | 28.76 | C |
| ATOM | 223 | N   | ARG | A | 44 | 18.725 | 28.103 | 9.419  | 1.00 | 30.34 | N |
| ATOM | 224 | CA  | ARG | A | 44 | 18.415 | 26.693 | 9.507  | 1.00 | 31.59 | C |
| ATOM | 225 | C   | ARG | A | 44 | 18.965 | 26.050 | 8.267  | 1.00 | 31.44 | C |
| ATOM | 226 | O   | ARG | A | 44 | 18.540 | 26.359 | 7.169  | 1.00 | 32.24 | O |
| ATOM | 227 | CB  | ARG | A | 44 | 16.923 | 26.399 | 9.502  | 1.00 | 32.07 | C |
| ATOM | 228 | CG  | ARG | A | 44 | 16.105 | 27.115 | 10.563 | 1.00 | 36.61 | C |
| ATOM | 229 | CD  | ARG | A | 44 | 14.638 | 26.534 | 10.809 | 1.00 | 39.09 | C |
| ATOM | 230 | NE  | ARG | A | 44 | 14.350 | 25.140 | 10.395 | 1.00 | 41.98 | N |
| ATOM | 231 | CZ  | ARG | A | 44 | 14.179 | 24.099 | 11.246 | 1.00 | 43.25 | C |
| ATOM | 232 | NH1 | ARG | A | 44 | 14.332 | 24.244 | 12.561 | 1.00 | 40.76 | N |
| ATOM | 233 | NH2 | ARG | A | 44 | 13.864 | 22.892 | 10.777 | 1.00 | 44.70 | N |
| ATOM | 234 | N   | LEU | A | 45 | 19.878 | 25.118 | 8.428  | 1.00 | 31.29 | N |
| ATOM | 235 | CA  | LEU | A | 45 | 20.544 | 24.560 | 7.294  | 1.00 | 30.82 | C |
| ATOM | 236 | C   | LEU | A | 45 | 20.744 | 23.083 | 7.470  | 1.00 | 31.52 | C |
| ATOM | 237 | O   | LEU | A | 45 | 20.690 | 22.550 | 8.597  | 1.00 | 31.99 | O |
| ATOM | 238 | CB  | LEU | A | 45 | 21.909 | 25.221 | 7.134  | 1.00 | 29.63 | C |
| ATOM | 239 | CG  | LEU | A | 45 | 21.873 | 26.697 | 6.813  | 1.00 | 31.00 | C |
| ATOM | 240 | CD1 | LEU | A | 45 | 23.279 | 27.338 | 7.030  | 1.00 | 31.79 | C |
| ATOM | 241 | CD2 | LEU | A | 45 | 21.403 | 26.918 | 5.378  | 1.00 | 31.14 | C |
| ATOM | 242 | N   | SER | A | 46 | 21.004 | 22.437 | 6.338  | 1.00 | 31.72 | N |
| ATOM | 243 | CA  | SER | A | 46 | 21.345 | 21.057 | 6.327  | 1.00 | 32.17 | C |
| ATOM | 244 | C   | SER | A | 46 | 22.771 | 20.978 | 6.767  | 1.00 | 32.55 | C |
| ATOM | 245 | O   | SER | A | 46 | 23.568 | 21.871 | 6.562  | 1.00 | 31.31 | O |
| ATOM | 246 | CB  | SER | A | 46 | 21.255 | 20.447 | 4.936  | 1.00 | 32.06 | C |
| ATOM | 247 | OG  | SER | A | 46 | 21.909 | 19.187 | 4.931  | 1.00 | 31.15 | O |
| ATOM | 248 | N   | GLN | A | 47 | 23.068 | 19.849 | 7.358  | 1.00 | 33.60 | N |
| ATOM | 249 | CA  | GLN | A | 47 | 24.370 | 19.546 | 7.878  | 1.00 | 34.42 | C |
| ATOM | 250 | C   | GLN | A | 47 | 25.385 | 19.453 | 6.754  | 1.00 | 34.74 | C |
| ATOM | 251 | O   | GLN | A | 47 | 26.554 | 19.685 | 6.971  | 1.00 | 35.40 | O |
| ATOM | 252 | CB  | GLN | A | 47 | 24.232 | 18.194 | 8.593  | 1.00 | 35.09 | C |
| ATOM | 253 | CG  | GLN | A | 47 | 25.465 | 17.417 | 8.733  | 1.00 | 36.19 | C |
| ATOM | 254 | CD  | GLN | A | 47 | 25.670 | 16.422 | 7.678  | 1.00 | 36.93 | C |
| ATOM | 255 | OE1 | GLN | A | 47 | 24.757 | 16.093 | 6.902  | 1.00 | 38.75 | O |
| ATOM | 256 | NE2 | GLN | A | 47 | 26.894 | 15.903 | 7.630  | 1.00 | 40.53 | N |
| ATOM | 257 | N   | SER | A | 48 | 24.933 | 19.095 | 5.556  | 1.00 | 34.63 | N |
| ATOM | 258 | CA  | SER | A | 48 | 25.821 | 18.922 | 4.415  | 1.00 | 34.93 | C |
| ATOM | 259 | C   | SER | A | 48 | 26.128 | 20.249 | 3.735  | 1.00 | 35.90 | C |
| ATOM | 260 | O   | SER | A | 48 | 26.990 | 20.315 | 2.862  | 1.00 | 36.31 | O |
| ATOM | 261 | CB  | SER | A | 48 | 25.182 | 17.991 | 3.381  | 1.00 | 34.59 | C |
| ATOM | 262 | OG  | SER | A | 48 | 23.912 | 18.483 | 2.955  | 1.00 | 33.48 | O |
| ATOM | 263 | N   | ASP | A | 49 | 25.415 | 21.302 | 4.124  | 1.00 | 36.41 | N |
| ATOM | 264 | CA  | ASP | A | 49 | 25.583 | 22.606 | 3.512  | 1.00 | 37.09 | C |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 265 | C   | ASP | A | 49 | 26.855 | 23.291 | 3.989  | 1.00 | 37.81 | C |
| ATOM | 266 | O   | ASP | A | 49 | 27.020 | 23.523 | 5.182  | 1.00 | 36.99 | O |
| ATOM | 267 | CB  | ASP | A | 49 | 24.383 | 23.451 | 3.877  | 1.00 | 37.42 | C |
| ATOM | 268 | CG  | ASP | A | 49 | 24.323 | 24.733 | 3.117  | 1.00 | 38.29 | C |
| ATOM | 269 | OD1 | ASP | A | 49 | 25.383 | 25.351 | 2.849  | 1.00 | 37.80 | O |
| ATOM | 270 | OD2 | ASP | A | 49 | 23.223 | 25.191 | 2.760  | 1.00 | 40.61 | O |
| ATOM | 271 | N   | PRO | A | 50 | 27.740 | 23.649 | 3.056  | 1.00 | 38.39 | N |
| ATOM | 272 | CA  | PRO | A | 50 | 29.005 | 24.291 | 3.409  | 1.00 | 38.24 | C |
| ATOM | 273 | C   | PRO | A | 50 | 28.802 | 25.502 | 4.285  | 1.00 | 38.16 | C |
| ATOM | 274 | O   | PRO | A | 50 | 29.671 | 25.797 | 5.088  | 1.00 | 37.37 | O |
| ATOM | 275 | CB  | PRO | A | 50 | 29.577 | 24.738 | 2.051  | 1.00 | 38.14 | C |
| ATOM | 276 | CG  | PRO | A | 50 | 28.978 | 23.915 | 1.070  | 1.00 | 38.31 | C |
| ATOM | 277 | CD  | PRO | A | 50 | 27.620 | 23.473 | 1.601  | 1.00 | 38.85 | C |
| ATOM | 278 | N   | ARG | A | 51 | 27.686 | 26.199 | 4.125  | 1.00 | 38.66 | N |
| ATOM | 279 | CA  | ARG | A | 51 | 27.448 | 27.403 | 4.912  | 1.00 | 39.05 | C |
| ATOM | 280 | C   | ARG | A | 51 | 27.332 | 27.077 | 6.391  | 1.00 | 38.94 | C |
| ATOM | 281 | O   | ARG | A | 51 | 27.668 | 27.908 | 7.259  | 1.00 | 38.35 | O |
| ATOM | 282 | CB  | ARG | A | 51 | 26.199 | 28.120 | 4.438  | 1.00 | 39.34 | C |
| ATOM | 283 | CG  | ARG | A | 51 | 26.372 | 28.781 | 3.067  | 1.00 | 41.10 | C |
| ATOM | 284 | CD  | ARG | A | 51 | 25.099 | 29.355 | 2.486  | 1.00 | 42.20 | C |
| ATOM | 285 | NE  | ARG | A | 51 | 24.111 | 28.314 | 2.192  | 1.00 | 44.96 | N |
| ATOM | 286 | CZ  | ARG | A | 51 | 22.815 | 28.551 | 2.043  | 1.00 | 46.68 | C |
| ATOM | 287 | NH1 | ARG | A | 51 | 22.348 | 29.795 | 2.162  | 1.00 | 47.61 | N |
| ATOM | 288 | NH2 | ARG | A | 51 | 21.980 | 27.563 | 1.774  | 1.00 | 46.08 | N |
| ATOM | 289 | N   | ALA | A | 52 | 26.882 | 25.867 | 6.688  | 1.00 | 38.31 | N |
| ATOM | 290 | CA  | ALA | A | 52 | 26.729 | 25.498 | 8.082  | 1.00 | 38.63 | C |
| ATOM | 291 | C   | ALA | A | 52 | 28.093 | 25.311 | 8.677  | 1.00 | 38.81 | C |
| ATOM | 292 | O   | ALA | A | 52 | 28.341 | 25.682 | 9.816  | 1.00 | 39.03 | O |
| ATOM | 293 | CB  | ALA | A | 52 | 25.907 | 24.233 | 8.235  | 1.00 | 38.36 | C |
| ATOM | 294 | N   | GLU | A | 53 | 28.988 | 24.733 | 7.899  | 1.00 | 39.48 | N |
| ATOM | 295 | CA  | GLU | A | 53 | 30.316 | 24.484 | 8.388  | 1.00 | 40.51 | C |
| ATOM | 296 | C   | GLU | A | 53 | 31.038 | 25.802 | 8.621  | 1.00 | 40.41 | C |
| ATOM | 297 | O   | GLU | A | 53 | 31.740 | 25.954 | 9.618  | 1.00 | 39.82 | O |
| ATOM | 298 | CB  | GLU | A | 53 | 31.093 | 23.614 | 7.436  | 1.00 | 40.70 | C |
| ATOM | 299 | CG  | GLU | A | 53 | 32.129 | 22.790 | 8.171  | 1.00 | 44.79 | C |
| ATOM | 300 | CD  | GLU | A | 53 | 31.596 | 21.435 | 8.633  | 1.00 | 48.98 | C |
| ATOM | 301 | OE1 | GLU | A | 53 | 30.427 | 21.329 | 9.017  | 1.00 | 51.56 | O |
| ATOM | 302 | OE2 | GLU | A | 53 | 32.354 | 20.454 | 8.620  | 1.00 | 54.44 | O |
| ATOM | 303 | N   | GLU | A | 54 | 30.851 | 26.752 | 7.713  | 1.00 | 40.45 | N |
| ATOM | 304 | CA  | GLU | A | 54 | 31.465 | 28.060 | 7.853  | 1.00 | 41.40 | C |
| ATOM | 305 | C   | GLU | A | 54 | 30.991 | 28.731 | 9.162  | 1.00 | 40.32 | C |
| ATOM | 306 | O   | GLU | A | 54 | 31.760 | 29.374 | 9.836  | 1.00 | 39.89 | O |
| ATOM | 307 | CB  | GLU | A | 54 | 31.119 | 28.974 | 6.679  | 1.00 | 42.12 | C |
| ATOM | 308 | CG  | GLU | A | 54 | 31.697 | 28.557 | 5.333  | 1.00 | 47.25 | C |
| ATOM | 309 | CD  | GLU | A | 54 | 30.953 | 29.191 | 4.129  | 1.00 | 53.54 | C |
| ATOM | 310 | OE1 | GLU | A | 54 | 30.459 | 30.366 | 4.276  | 1.00 | 57.47 | O |
| ATOM | 311 | OE2 | GLU | A | 54 | 30.882 | 28.527 | 3.036  | 1.00 | 53.82 | O |
| ATOM | 312 | N   | LEU | A | 55 | 29.735 | 28.534 | 9.533  | 1.00 | 39.03 | N |
| ATOM | 313 | CA  | LEU | A | 55 | 29.223 | 29.198 | 10.687 | 1.00 | 37.80 | C |
| ATOM | 314 | C   | LEU | A | 55 | 29.840 | 28.673 | 11.956 | 1.00 | 36.83 | C |
| ATOM | 315 | O   | LEU | A | 55 | 30.293 | 29.464 | 12.795 | 1.00 | 35.66 | O |
| ATOM | 316 | CB  | LEU | A | 55 | 27.715 | 29.081 | 10.725 | 1.00 | 38.06 | C |
| ATOM | 317 | CG  | LEU | A | 55 | 27.072 | 29.921 | 9.621  | 1.00 | 37.63 | C |
| ATOM | 318 | CD1 | LEU | A | 55 | 25.620 | 29.569 | 9.449  | 1.00 | 39.63 | C |
| ATOM | 319 | CD2 | LEU | A | 55 | 27.174 | 31.356 | 9.928  | 1.00 | 36.27 | C |
| ATOM | 320 | N   | ILE | A | 56 | 29.876 | 27.346 | 12.079 | 1.00 | 35.87 | N |
| ATOM | 321 | CA  | ILE | A | 56 | 30.436 | 26.684 | 13.257 | 1.00 | 35.35 | C |
| ATOM | 322 | C   | ILE | A | 56 | 31.916 | 27.001 | 13.410 | 1.00 | 35.82 | C |
| ATOM | 323 | O   | ILE | A | 56 | 32.377 | 27.299 | 14.499 | 1.00 | 36.59 | O |
| ATOM | 324 | CB  | ILE | A | 56 | 30.281 | 25.198 | 13.139 | 1.00 | 34.84 | C |
| ATOM | 325 | CG1 | ILE | A | 56 | 28.790 | 24.810 | 13.132 | 1.00 | 34.00 | C |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 326 | CG2 | ILE | A | 56 | 31.022 | 24.535 | 14.280 | 1.00 | 34.89 | C |
| ATOM | 327 | CD1 | ILE | A | 56 | 28.502 | 23.361 | 12.684 | 1.00 | 30.65 | C |
| ATOM | 328 | N   | GLU | A | 57 | 32.636 | 26.964 | 12.301 | 1.00 | 36.28 | N |
| ATOM | 329 | CA  | GLU | A | 57 | 34.056 | 27.244 | 12.255 | 1.00 | 37.26 | C |
| ATOM | 330 | C   | GLU | A | 57 | 34.295 | 28.634 | 12.809 | 1.00 | 37.41 | C |
| ATOM | 331 | O   | GLU | A | 57 | 35.278 | 28.879 | 13.516 | 1.00 | 38.73 | O |
| ATOM | 332 | CB  | GLU | A | 57 | 34.562 | 27.167 | 10.795 | 1.00 | 37.54 | C |
| ATOM | 333 | CG  | GLU | A | 57 | 36.035 | 27.462 | 10.572 | 1.00 | 39.41 | C |
| ATOM | 334 | CD  | GLU | A | 57 | 36.948 | 26.668 | 11.493 | 1.00 | 44.86 | C |
| ATOM | 335 | OE1 | GLU | A | 57 | 36.666 | 25.458 | 11.741 | 1.00 | 48.72 | O |
| ATOM | 336 | OE2 | GLU | A | 57 | 37.961 | 27.260 | 11.965 | 1.00 | 46.32 | O |
| ATOM | 337 | N   | ASN | A | 58 | 33.386 | 29.537 | 12.485 | 1.00 | 36.64 | N |
| ATOM | 338 | CA  | ASN | A | 58 | 33.456 | 30.907 | 12.926 | 1.00 | 36.26 | C |
| ATOM | 339 | C   | ASN | A | 58 | 32.768 | 31.226 | 14.219 | 1.00 | 35.28 | C |
| ATOM | 340 | O   | ASN | A | 58 | 32.569 | 32.376 | 14.531 | 1.00 | 33.45 | O |
| ATOM | 341 | CB  | ASN | A | 58 | 32.798 | 31.758 | 11.898 | 1.00 | 36.88 | C |
| ATOM | 342 | CG  | ASN | A | 58 | 33.763 | 32.461 | 11.107 | 1.00 | 39.77 | C |
| ATOM | 343 | OD1 | ASN | A | 58 | 34.140 | 31.983 | 10.018 | 1.00 | 41.34 | O |
| ATOM | 344 | ND2 | ASN | A | 58 | 34.241 | 33.617 | 11.639 | 1.00 | 41.14 | N |
| ATOM | 345 | N   | GLU | A | 59 | 32.366 | 30.205 | 14.945 | 1.00 | 35.05 | N |
| ATOM | 346 | CA  | GLU | A | 59 | 31.706 | 30.415 | 16.226 | 1.00 | 35.00 | C |
| ATOM | 347 | C   | GLU | A | 59 | 30.481 | 31.314 | 16.133 | 1.00 | 33.86 | C |
| ATOM | 348 | O   | GLU | A | 59 | 30.293 | 32.238 | 16.904 | 1.00 | 33.16 | O |
| ATOM | 349 | CB  | GLU | A | 59 | 32.729 | 30.855 | 17.244 | 1.00 | 34.95 | C |
| ATOM | 350 | CG  | GLU | A | 59 | 33.708 | 29.700 | 17.423 | 1.00 | 37.79 | C |
| ATOM | 351 | CD  | GLU | A | 59 | 34.652 | 29.820 | 18.586 | 1.00 | 39.57 | C |
| ATOM | 352 | OE1 | GLU | A | 59 | 35.809 | 30.145 | 18.349 | 1.00 | 43.67 | O |
| ATOM | 353 | OE2 | GLU | A | 59 | 34.254 | 29.545 | 19.723 | 1.00 | 45.29 | O |
| ATOM | 354 | N   | GLU | A | 60 | 29.644 | 30.995 | 15.157 | 1.00 | 32.92 | N |
| ATOM | 355 | CA  | GLU | A | 60 | 28.359 | 31.641 | 14.983 | 1.00 | 32.66 | C |
| ATOM | 356 | C   | GLU | A | 60 | 27.284 | 30.576 | 14.993 | 1.00 | 30.59 | C |
| ATOM | 357 | O   | GLU | A | 60 | 27.456 | 29.485 | 14.461 | 1.00 | 30.47 | O |
| ATOM | 358 | CB  | GLU | A | 60 | 28.312 | 32.400 | 13.685 | 1.00 | 33.20 | C |
| ATOM | 359 | CG  | GLU | A | 60 | 29.384 | 33.454 | 13.615 | 1.00 | 38.62 | C |
| ATOM | 360 | CD  | GLU | A | 60 | 28.955 | 34.617 | 12.762 | 1.00 | 45.73 | C |
| ATOM | 361 | OE1 | GLU | A | 60 | 29.075 | 34.553 | 11.519 | 1.00 | 48.47 | O |
| ATOM | 362 | OE2 | GLU | A | 60 | 28.466 | 35.587 | 13.367 | 1.00 | 53.89 | O |
| ATOM | 363 | N   | PRO | A | 61 | 26.152 | 30.915 | 15.560 | 1.00 | 28.63 | N |
| ATOM | 364 | CA  | PRO | A | 61 | 25.073 | 29.954 | 15.735 | 1.00 | 28.05 | C |
| ATOM | 365 | C   | PRO | A | 61 | 24.462 | 29.451 | 14.443 | 1.00 | 27.61 | C |
| ATOM | 366 | O   | PRO | A | 61 | 24.475 | 30.120 | 13.426 | 1.00 | 27.23 | O |
| ATOM | 367 | CB  | PRO | A | 61 | 24.021 | 30.754 | 16.492 | 1.00 | 28.67 | C |
| ATOM | 368 | CG  | PRO | A | 61 | 24.385 | 32.140 | 16.400 | 1.00 | 27.46 | C |
| ATOM | 369 | CD  | PRO | A | 61 | 25.811 | 32.253 | 16.038 | 1.00 | 27.71 | C |
| ATOM | 370 | N   | VAL | A | 62 | 23.936 | 28.237 | 14.475 | 1.00 | 27.43 | N |
| ATOM | 371 | CA  | VAL | A | 62 | 23.254 | 27.685 | 13.317 | 1.00 | 27.09 | C |
| ATOM | 372 | C   | VAL | A | 62 | 22.372 | 26.569 | 13.802 | 1.00 | 27.40 | C |
| ATOM | 373 | O   | VAL | A | 62 | 22.707 | 25.893 | 14.780 | 1.00 | 27.79 | O |
| ATOM | 374 | CB  | VAL | A | 62 | 24.219 | 27.181 | 12.270 | 1.00 | 27.04 | C |
| ATOM | 375 | CG1 | VAL | A | 62 | 25.106 | 26.166 | 12.829 | 1.00 | 27.34 | C |
| ATOM | 376 | CG2 | VAL | A | 62 | 23.473 | 26.659 | 11.037 | 1.00 | 27.58 | C |
| ATOM | 377 | N   | VAL | A | 63 | 21.195 | 26.440 | 13.199 | 1.00 | 27.19 | N |
| ATOM | 378 | CA  | VAL | A | 63 | 20.339 | 25.338 | 13.526 | 1.00 | 27.37 | C |
| ATOM | 379 | C   | VAL | A | 63 | 20.540 | 24.324 | 12.383 | 1.00 | 27.33 | C |
| ATOM | 380 | O   | VAL | A | 63 | 20.360 | 24.672 | 11.208 | 1.00 | 27.05 | O |
| ATOM | 381 | CB  | VAL | A | 63 | 18.857 | 25.737 | 13.611 | 1.00 | 27.47 | C |
| ATOM | 382 | CG1 | VAL | A | 63 | 17.976 | 24.446 | 13.695 | 1.00 | 28.55 | C |
| ATOM | 383 | CG2 | VAL | A | 63 | 18.616 | 26.603 | 14.793 | 1.00 | 25.77 | C |
| ATOM | 384 | N   | LEU | A | 64 | 20.933 | 23.114 | 12.743 | 1.00 | 27.26 | N |
| ATOM | 385 | CA  | LEU | A | 64 | 21.119 | 22.001 | 11.820 | 1.00 | 28.51 | C |
| ATOM | 386 | C   | LEU | A | 64 | 19.897 | 21.128 | 11.894 | 1.00 | 28.40 | C |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 387 | O   | LEU | A | 64 | 19.517 | 20.692 | 12.982 | 1.00 | 28.69 | O |
| ATOM | 388 | CB  | LEU | A | 64 | 22.352 | 21.187 | 12.204 | 1.00 | 28.92 | C |
| ATOM | 389 | CG  | LEU | A | 64 | 23.624 | 22.016 | 12.142 | 1.00 | 31.65 | C |
| ATOM | 390 | CD1 | LEU | A | 64 | 24.800 | 21.273 | 12.534 | 1.00 | 34.84 | C |
| ATOM | 391 | CD2 | LEU | A | 64 | 23.843 | 22.490 | 10.722 | 1.00 | 35.77 | C |
| ATOM | 392 | N   | THR | A | 65 | 19.284 | 20.868 | 10.752 | 1.00 | 28.44 | N |
| ATOM | 393 | CA  | THR | A | 65 | 18.003 | 20.164 | 10.721 | 1.00 | 29.54 | C |
| ATOM | 394 | C   | THR | A | 65 | 18.054 | 18.659 | 10.534 | 1.00 | 29.40 | C |
| ATOM | 395 | O   | THR | A | 65 | 17.046 | 17.985 | 10.799 | 1.00 | 29.20 | O |
| ATOM | 396 | CB  | THR | A | 65 | 17.139 | 20.679 | 9.552  | 1.00 | 30.07 | C |
| ATOM | 397 | OG1 | THR | A | 65 | 17.879 | 20.569 | 8.318  | 1.00 | 30.75 | O |
| ATOM | 398 | CG2 | THR | A | 65 | 16.878 | 22.137 | 9.665  | 1.00 | 31.86 | C |
| ATOM | 399 | N   | ASP | A | 66 | 19.183 | 18.150 | 10.059 | 1.00 | 29.30 | N |
| ATOM | 400 | CA  | ASP | A | 66 | 19.323 | 16.722 | 9.719  | 1.00 | 29.78 | C |
| ATOM | 401 | C   | ASP | A | 66 | 20.573 | 15.970 | 10.196 | 1.00 | 29.12 | C |
| ATOM | 402 | O   | ASP | A | 66 | 21.081 | 15.141 | 9.432  | 1.00 | 29.09 | O |
| ATOM | 403 | CB  | ASP | A | 66 | 19.301 | 16.582 | 8.195  | 1.00 | 29.41 | C |
| ATOM | 404 | CG  | ASP | A | 66 | 20.274 | 17.507 | 7.525  | 1.00 | 32.36 | C |
| ATOM | 405 | OD1 | ASP | A | 66 | 20.924 | 18.319 | 8.230  | 1.00 | 34.87 | O |
| ATOM | 406 | OD2 | ASP | A | 66 | 20.447 | 17.534 | 6.287  | 1.00 | 35.70 | O |
| ATOM | 407 | N   | THR | A | 67 | 21.078 | 16.254 | 11.404 | 1.00 | 28.05 | N |
| ATOM | 408 | CA  | THR | A | 67 | 22.266 | 15.565 | 11.897 | 1.00 | 27.24 | C |
| ATOM | 409 | C   | THR | A | 67 | 21.943 | 14.171 | 12.355 | 1.00 | 26.92 | C |
| ATOM | 410 | O   | THR | A | 67 | 22.807 | 13.297 | 12.367 | 1.00 | 25.98 | O |
| ATOM | 411 | CB  | THR | A | 67 | 22.856 | 16.258 | 13.134 | 1.00 | 27.78 | C |
| ATOM | 412 | OG1 | THR | A | 67 | 21.874 | 16.338 | 14.186 | 1.00 | 25.71 | O |
| ATOM | 413 | CG2 | THR | A | 67 | 23.268 | 17.664 | 12.820 | 1.00 | 29.22 | C |
| ATOM | 414 | N   | ASN | A | 68 | 20.704 | 13.979 | 12.777 | 1.00 | 26.53 | N |
| ATOM | 415 | CA  | ASN | A | 68 | 20.307 | 12.711 | 13.355 | 1.00 | 27.10 | C |
| ATOM | 416 | C   | ASN | A | 68 | 21.075 | 12.499 | 14.647 | 1.00 | 26.46 | C |
| ATOM | 417 | O   | ASN | A | 68 | 21.223 | 11.399 | 15.092 | 1.00 | 26.90 | O |
| ATOM | 418 | CB  | ASN | A | 68 | 20.583 | 11.547 | 12.401 | 1.00 | 27.41 | C |
| ATOM | 419 | CG  | ASN | A | 68 | 19.546 | 11.415 | 11.308 | 1.00 | 28.18 | C |
| ATOM | 420 | OD1 | ASN | A | 68 | 18.345 | 11.286 | 11.566 | 1.00 | 29.22 | O |
| ATOM | 421 | ND2 | ASN | A | 68 | 20.006 | 11.445 | 10.077 | 1.00 | 29.40 | N |
| ATOM | 422 | N   | LEU | A | 69 | 21.585 | 13.569 | 15.227 | 1.00 | 26.58 | N |
| ATOM | 423 | CA  | LEU | A | 69 | 22.429 | 13.481 | 16.427 | 1.00 | 26.67 | C |
| ATOM | 424 | C   | LEU | A | 69 | 21.832 | 12.639 | 17.558 | 1.00 | 26.73 | C |
| ATOM | 425 | O   | LEU | A | 69 | 22.550 | 11.822 | 18.166 | 1.00 | 27.74 | O |
| ATOM | 426 | CB  | LEU | A | 69 | 22.739 | 14.870 | 16.968 | 1.00 | 26.04 | C |
| ATOM | 427 | CG  | LEU | A | 69 | 23.677 | 14.904 | 18.157 | 1.00 | 26.23 | C |
| ATOM | 428 | CD1 | LEU | A | 69 | 24.986 | 14.168 | 17.894 | 1.00 | 27.92 | C |
| ATOM | 429 | CD2 | LEU | A | 69 | 23.976 | 16.343 | 18.556 | 1.00 | 24.74 | C |
| ATOM | 430 | N   | VAL | A | 70 | 20.557 | 12.857 | 17.861 | 1.00 | 26.02 | N |
| ATOM | 431 | CA  | VAL | A | 70 | 19.882 | 12.091 | 18.898 | 1.00 | 26.50 | C |
| ATOM | 432 | C   | VAL | A | 70 | 18.673 | 11.364 | 18.345 | 1.00 | 26.71 | C |
| ATOM | 433 | O   | VAL | A | 70 | 17.650 | 11.183 | 19.015 | 1.00 | 25.59 | O |
| ATOM | 434 | CB  | VAL | A | 70 | 19.479 | 12.943 | 20.098 | 1.00 | 26.46 | C |
| ATOM | 435 | CG1 | VAL | A | 70 | 20.717 | 13.505 | 20.764 | 1.00 | 28.17 | C |
| ATOM | 436 | CG2 | VAL | A | 70 | 18.517 | 14.016 | 19.716 | 1.00 | 23.88 | C |
| ATOM | 437 | N   | TYR | A | 71 | 18.832 | 10.920 | 17.113 | 1.00 | 27.86 | N |
| ATOM | 438 | CA  | TYR | A | 71 | 17.791 | 10.159 | 16.451 | 1.00 | 29.60 | C |
| ATOM | 439 | C   | TYR | A | 71 | 17.093 | 9.167  | 17.388 | 1.00 | 29.76 | C |
| ATOM | 440 | O   | TYR | A | 71 | 15.905 | 9.202  | 17.478 | 1.00 | 30.54 | O |
| ATOM | 441 | CB  | TYR | A | 71 | 18.326 | 9.459  | 15.208 | 1.00 | 29.31 | C |
| ATOM | 442 | CG  | TYR | A | 71 | 17.347 | 8.479  | 14.686 | 1.00 | 31.42 | C |
| ATOM | 443 | CD1 | TYR | A | 71 | 16.136 | 8.884  | 14.120 | 1.00 | 31.39 | C |
| ATOM | 444 | CD2 | TYR | A | 71 | 17.610 | 7.107  | 14.779 | 1.00 | 32.30 | C |
| ATOM | 445 | CE1 | TYR | A | 71 | 15.223 | 7.905  | 13.641 | 1.00 | 31.86 | C |
| ATOM | 446 | CE2 | TYR | A | 71 | 16.736 | 6.181  | 14.317 | 1.00 | 29.75 | C |
| ATOM | 447 | CZ  | TYR | A | 71 | 15.556 | 6.558  | 13.755 | 1.00 | 31.10 | C |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 448 | OH  | TYR | A | 71 | 14.698 | 5.530  | 13.342 | 1.00 | 39.44 | O |
| ATOM | 449 | N   | PRO | A | 72 | 17.807 | 8.317  | 18.108 | 1.00 | 30.56 | N |
| ATOM | 450 | CA  | PRO | A | 72 | 17.150 | 7.336  | 18.991 | 1.00 | 30.85 | C |
| ATOM | 451 | C   | PRO | A | 72 | 16.389 | 7.914  | 20.158 | 1.00 | 30.85 | C |
| ATOM | 452 | O   | PRO | A | 72 | 15.549 | 7.233  | 20.750 | 1.00 | 30.12 | O |
| ATOM | 453 | CB  | PRO | A | 72 | 18.310 | 6.468  | 19.507 | 1.00 | 30.71 | C |
| ATOM | 454 | CG  | PRO | A | 72 | 19.420 | 6.692  | 18.515 | 1.00 | 31.79 | C |
| ATOM | 455 | CD  | PRO | A | 72 | 19.268 | 8.158  | 18.096 | 1.00 | 30.88 | C |
| ATOM | 456 | N   | ALA | A | 73 | 16.650 | 9.166  | 20.508 | 1.00 | 31.72 | N |
| ATOM | 457 | CA  | ALA | A | 73 | 15.918 | 9.743  | 21.627 | 1.00 | 31.71 | C |
| ATOM | 458 | C   | ALA | A | 73 | 14.596 | 10.371 | 21.172 | 1.00 | 31.83 | C |
| ATOM | 459 | O   | ALA | A | 73 | 13.786 | 10.808 | 22.000 | 1.00 | 31.52 | O |
| ATOM | 460 | CB  | ALA | A | 73 | 16.762 | 10.742 | 22.340 | 1.00 | 32.17 | C |
| ATOM | 461 | N   | LEU | A | 74 | 14.345 | 10.408 | 19.868 | 1.00 | 31.19 | N |
| ATOM | 462 | CA  | LEU | A | 74 | 13.108 | 11.028 | 19.439 | 1.00 | 32.01 | C |
| ATOM | 463 | C   | LEU | A | 74 | 11.856 | 10.343 | 19.965 | 1.00 | 32.30 | C |
| ATOM | 464 | O   | LEU | A | 74 | 10.807 | 10.914 | 19.963 | 1.00 | 31.90 | O |
| ATOM | 465 | CB  | LEU | A | 74 | 13.050 | 11.191 | 17.931 | 1.00 | 31.25 | C |
| ATOM | 466 | CG  | LEU | A | 74 | 14.140 | 12.103 | 17.400 | 1.00 | 34.53 | C |
| ATOM | 467 | CD1 | LEU | A | 74 | 13.904 | 12.418 | 15.965 | 1.00 | 37.35 | C |
| ATOM | 468 | CD2 | LEU | A | 74 | 14.264 | 13.436 | 18.200 | 1.00 | 34.44 | C |
| ATOM | 469 | N   | LYS | A | 75 | 11.963 | 9.100  | 20.396 | 1.00 | 34.18 | N |
| ATOM | 470 | CA  | LYS | A | 75 | 10.802 | 8.376  | 20.910 | 1.00 | 34.36 | C |
| ATOM | 471 | C   | LYS | A | 75 | 10.618 | 8.616  | 22.403 | 1.00 | 35.18 | C |
| ATOM | 472 | O   | LYS | A | 75 | 9.575  | 8.304  | 22.945 | 1.00 | 35.70 | O |
| ATOM | 473 | CB  | LYS | A | 75 | 10.950 | 6.876  | 20.631 | 1.00 | 34.51 | C |
| ATOM | 474 | CG  | LYS | A | 75 | 12.138 | 6.219  | 21.294 | 1.00 | 33.19 | C |
| ATOM | 475 | CD  | LYS | A | 75 | 12.302 | 4.754  | 20.834 | 1.00 | 31.54 | C |
| ATOM | 476 | CE  | LYS | A | 75 | 13.796 | 4.304  | 20.744 | 1.00 | 29.70 | C |
| ATOM | 477 | NZ  | LYS | A | 75 | 14.460 | 4.158  | 22.026 | 1.00 | 28.79 | N |
| ATOM | 478 | N   | TRP | A | 76 | 11.619 | 9.181  | 23.071 | 1.00 | 35.44 | N |
| ATOM | 479 | CA  | TRP | A | 76 | 11.517 | 9.426  | 24.495 | 1.00 | 36.05 | C |
| ATOM | 480 | C   | TRP | A | 76 | 10.307 | 10.264 | 24.893 | 1.00 | 37.47 | C |
| ATOM | 481 | O   | TRP | A | 76 | 9.958  | 11.222 | 24.212 | 1.00 | 38.43 | O |
| ATOM | 482 | CB  | TRP | A | 76 | 12.742 | 10.179 | 24.994 | 1.00 | 35.67 | C |
| ATOM | 483 | CG  | TRP | A | 76 | 13.980 | 9.395  | 24.963 | 1.00 | 33.87 | C |
| ATOM | 484 | CD1 | TRP | A | 76 | 14.136 | 8.116  | 24.520 | 1.00 | 32.29 | C |
| ATOM | 485 | CD2 | TRP | A | 76 | 15.252 | 9.821  | 25.409 | 1.00 | 30.36 | C |
| ATOM | 486 | NE1 | TRP | A | 76 | 15.440 | 7.723  | 24.673 | 1.00 | 30.42 | N |
| ATOM | 487 | CE2 | TRP | A | 76 | 16.143 | 8.754  | 25.221 | 1.00 | 28.82 | C |
| ATOM | 488 | CE3 | TRP | A | 76 | 15.739 | 11.013 | 25.954 | 1.00 | 29.45 | C |
| ATOM | 489 | CZ2 | TRP | A | 76 | 17.471 | 8.833  | 25.560 | 1.00 | 30.56 | C |
| ATOM | 490 | CZ3 | TRP | A | 76 | 17.056 | 11.091 | 26.291 | 1.00 | 29.56 | C |
| ATOM | 491 | CH2 | TRP | A | 76 | 17.917 | 10.017 | 26.092 | 1.00 | 30.20 | C |
| ATOM | 492 | N   | ASP | A | 77 | 9.698  | 9.894  | 26.014 | 1.00 | 38.14 | N |
| ATOM | 493 | CA  | ASP | A | 77 | 8.620  | 10.640 | 26.635 | 1.00 | 38.33 | C |
| ATOM | 494 | C   | ASP | A | 77 | 8.653  | 10.223 | 28.094 | 1.00 | 37.89 | C |
| ATOM | 495 | O   | ASP | A | 77 | 9.443  | 9.390  | 28.447 | 1.00 | 37.97 | O |
| ATOM | 496 | CB  | ASP | A | 77 | 7.283  | 10.353 | 25.974 | 1.00 | 38.71 | C |
| ATOM | 497 | CG  | ASP | A | 77 | 6.882  | 8.904  | 26.049 | 1.00 | 39.50 | C |
| ATOM | 498 | OD1 | ASP | A | 77 | 7.414  | 8.107  | 26.867 | 1.00 | 41.50 | O |
| ATOM | 499 | OD2 | ASP | A | 77 | 6.006  | 8.472  | 25.299 | 1.00 | 41.98 | O |
| ATOM | 500 | N   | LEU | A | 78 | 7.838  | 10.800 | 28.955 | 1.00 | 38.47 | N |
| ATOM | 501 | CA  | LEU | A | 78 | 7.941  | 10.481 | 30.375 | 1.00 | 39.09 | C |
| ATOM | 502 | C   | LEU | A | 78 | 7.734  | 9.002  | 30.662 | 1.00 | 39.89 | C |
| ATOM | 503 | O   | LEU | A | 78 | 8.421  | 8.423  | 31.507 | 1.00 | 40.19 | O |
| ATOM | 504 | CB  | LEU | A | 78 | 6.966  | 11.310 | 31.171 | 1.00 | 39.02 | C |
| ATOM | 505 | CG  | LEU | A | 78 | 7.169  | 12.815 | 31.042 | 1.00 | 41.51 | C |
| ATOM | 506 | CD1 | LEU | A | 78 | 6.058  | 13.567 | 31.764 | 1.00 | 42.72 | C |
| ATOM | 507 | CD2 | LEU | A | 78 | 8.522  | 13.216 | 31.618 | 1.00 | 42.31 | C |
| ATOM | 508 | N   | GLU | A | 79 | 6.795  | 8.369  | 29.971 | 1.00 | 40.66 | N |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 509 | CA  | GLU | A | 79 | 6.557  | 6.948  | 30.212 | 1.00 | 41.43 | C |
| ATOM | 510 | C   | GLU | A | 79 | 7.794  | 6.086  | 29.909 | 1.00 | 40.84 | C |
| ATOM | 511 | O   | GLU | A | 79 | 8.228  | 5.283  | 30.742 | 1.00 | 40.45 | O |
| ATOM | 512 | CB  | GLU | A | 79 | 5.343  | 6.458  | 29.418 | 1.00 | 42.10 | C |
| ATOM | 513 | CG  | GLU | A | 79 | 5.023  | 4.998  | 29.658 | 1.00 | 45.06 | C |
| ATOM | 514 | CD  | GLU | A | 79 | 3.840  | 4.525  | 28.846 | 1.00 | 49.74 | C |
| ATOM | 515 | OE1 | GLU | A | 79 | 3.436  | 5.254  | 27.914 | 1.00 | 52.37 | O |
| ATOM | 516 | OE2 | GLU | A | 79 | 3.316  | 3.426  | 29.150 | 1.00 | 53.21 | O |
| ATOM | 517 | N   | TYR | A | 80 | 8.361  | 6.248  | 28.718 | 1.00 | 40.43 | N |
| ATOM | 518 | CA  | TYR | A | 80 | 9.559  | 5.495  | 28.362 | 1.00 | 40.14 | C |
| ATOM | 519 | C   | TYR | A | 80 | 10.750 | 5.765  | 29.297 | 1.00 | 40.06 | C |
| ATOM | 520 | O   | TYR | A | 80 | 11.485 | 4.844  | 29.664 | 1.00 | 39.72 | O |
| ATOM | 521 | CB  | TYR | A | 80 | 9.946  | 5.832  | 26.946 | 1.00 | 39.96 | C |
| ATOM | 522 | CG  | TYR | A | 80 | 11.193 | 5.147  | 26.420 | 1.00 | 39.51 | C |
| ATOM | 523 | CD1 | TYR | A | 80 | 11.118 | 3.897  | 25.804 | 1.00 | 38.93 | C |
| ATOM | 524 | CD2 | TYR | A | 80 | 12.433 | 5.768  | 26.490 | 1.00 | 36.89 | C |
| ATOM | 525 | CE1 | TYR | A | 80 | 12.253 | 3.277  | 25.290 | 1.00 | 38.08 | C |
| ATOM | 526 | CE2 | TYR | A | 80 | 13.562 | 5.154  | 25.993 | 1.00 | 38.15 | C |
| ATOM | 527 | CZ  | TYR | A | 80 | 13.468 | 3.915  | 25.379 | 1.00 | 39.06 | C |
| ATOM | 528 | OH  | TYR | A | 80 | 14.604 | 3.319  | 24.863 | 1.00 | 38.99 | O |
| ATOM | 529 | N   | LEU | A | 81 | 10.935 | 7.017  | 29.688 | 1.00 | 39.68 | N |
| ATOM | 530 | CA  | LEU | A | 81 | 12.061 | 7.362  | 30.565 | 1.00 | 40.01 | C |
| ATOM | 531 | C   | LEU | A | 81 | 11.858 | 6.806  | 31.978 | 1.00 | 39.86 | C |
| ATOM | 532 | O   | LEU | A | 81 | 12.792 | 6.284  | 32.608 | 1.00 | 39.47 | O |
| ATOM | 533 | CB  | LEU | A | 81 | 12.314 | 8.889  | 30.604 | 1.00 | 39.50 | C |
| ATOM | 534 | CG  | LEU | A | 81 | 12.765 | 9.532  | 29.287 | 1.00 | 39.76 | C |
| ATOM | 535 | CD1 | LEU | A | 81 | 12.805 | 11.045 | 29.402 | 1.00 | 39.84 | C |
| ATOM | 536 | CD2 | LEU | A | 81 | 14.117 | 9.018  | 28.840 | 1.00 | 39.32 | C |
| ATOM | 537 | N   | GLN | A | 82 | 10.645 | 6.932  | 32.482 | 1.00 | 40.38 | N |
| ATOM | 538 | CA  | GLN | A | 82 | 10.346 | 6.415  | 33.804 | 1.00 | 41.02 | C |
| ATOM | 539 | C   | GLN | A | 82 | 10.612 | 4.920  | 33.799 | 1.00 | 40.84 | C |
| ATOM | 540 | O   | GLN | A | 82 | 11.193 | 4.379  | 34.711 | 1.00 | 40.35 | O |
| ATOM | 541 | CB  | GLN | A | 82 | 8.900  | 6.688  | 34.164 | 1.00 | 41.40 | C |
| ATOM | 542 | CG  | GLN | A | 82 | 8.447  | 5.906  | 35.351 | 1.00 | 42.97 | C |
| ATOM | 543 | CD  | GLN | A | 82 | 7.291  | 6.560  | 36.099 | 1.00 | 45.14 | C |
| ATOM | 544 | OE1 | GLN | A | 82 | 6.662  | 7.502  | 35.616 | 1.00 | 44.10 | O |
| ATOM | 545 | NE2 | GLN | A | 82 | 7.003  | 6.039  | 37.287 | 1.00 | 48.04 | N |
| ATOM | 546 | N   | GLU | A | 83 | 10.222 | 4.256  | 32.728 | 1.00 | 41.35 | N |
| ATOM | 547 | CA  | GLU | A | 83 | 10.442 | 2.816  | 32.620 | 1.00 | 41.46 | C |
| ATOM | 548 | C   | GLU | A | 83 | 11.926 | 2.444  | 32.465 | 1.00 | 40.81 | C |
| ATOM | 549 | O   | GLU | A | 83 | 12.350 | 1.407  | 32.958 | 1.00 | 41.13 | O |
| ATOM | 550 | CB  | GLU | A | 83 | 9.610  | 2.243  | 31.472 | 1.00 | 41.27 | C |
| ATOM | 551 | CG  | GLU | A | 83 | 9.609  | 0.728  | 31.366 | 1.00 | 44.77 | C |
| ATOM | 552 | CD  | GLU | A | 83 | 8.878  | 0.018  | 32.514 | 1.00 | 49.16 | C |
| ATOM | 553 | OE1 | GLU | A | 83 | 8.219  | 0.672  | 33.347 | 1.00 | 52.26 | O |
| ATOM | 554 | OE2 | GLU | A | 83 | 8.978  | -1.220 | 32.606 | 1.00 | 53.23 | O |
| ATOM | 555 | N   | ASN | A | 84 | 12.743 | 3.298  | 31.854 | 1.00 | 39.81 | N |
| ATOM | 556 | CA  | ASN | A | 84 | 14.099 | 2.859  | 31.515 | 1.00 | 38.82 | C |
| ATOM | 557 | C   | ASN | A | 84 | 15.290 | 3.611  | 32.048 | 1.00 | 38.20 | C |
| ATOM | 558 | O   | ASN | A | 84 | 16.402 | 3.117  | 31.919 | 1.00 | 36.98 | O |
| ATOM | 559 | CB  | ASN | A | 84 | 14.244 | 2.828  | 29.995 | 1.00 | 38.83 | C |
| ATOM | 560 | CG  | ASN | A | 84 | 13.301 | 1.865  | 29.349 | 1.00 | 38.45 | C |
| ATOM | 561 | OD1 | ASN | A | 84 | 13.307 | 0.670  | 29.664 | 1.00 | 40.40 | O |
| ATOM | 562 | ND2 | ASN | A | 84 | 12.480 | 2.365  | 28.441 | 1.00 | 35.77 | N |
| ATOM | 563 | N   | ILE | A | 85 | 15.088 | 4.781  | 32.645 | 1.00 | 38.08 | N |
| ATOM | 564 | CA  | ILE | A | 85 | 16.226 | 5.598  | 32.998 | 1.00 | 38.57 | C |
| ATOM | 565 | C   | ILE | A | 85 | 16.929 | 5.280  | 34.307 | 1.00 | 38.70 | C |
| ATOM | 566 | O   | ILE | A | 85 | 17.849 | 5.993  | 34.702 | 1.00 | 39.78 | O |
| ATOM | 567 | CB  | ILE | A | 85 | 15.827 | 7.056  | 32.932 | 1.00 | 39.02 | C |
| ATOM | 568 | CG1 | ILE | A | 85 | 17.001 | 7.891  | 32.418 | 1.00 | 39.43 | C |
| ATOM | 569 | CG2 | ILE | A | 85 | 15.291 | 7.544  | 34.266 | 1.00 | 39.22 | C |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 570 | CD1 | ILE | A | 85 | 16.618 | 9.347  | 32.148 | 1.00 | 40.41 | C |
| ATOM | 571 | N   | GLY | A | 86 | 16.513 | 4.227  | 34.993 | 1.00 | 38.59 | N |
| ATOM | 572 | CA  | GLY | A | 86 | 17.208 | 3.801  | 36.199 | 1.00 | 38.15 | C |
| ATOM | 573 | C   | GLY | A | 86 | 16.658 | 4.386  | 37.476 | 1.00 | 37.92 | C |
| ATOM | 574 | O   | GLY | A | 86 | 15.652 | 5.097  | 37.461 | 1.00 | 37.90 | O |
| ATOM | 575 | N   | ASN | A | 87 | 17.359 | 4.113  | 38.574 | 1.00 | 37.70 | N |
| ATOM | 576 | CA  | ASN | A | 87 | 16.941 | 4.542  | 39.899 | 1.00 | 37.34 | C |
| ATOM | 577 | C   | ASN | A | 87 | 17.898 | 5.576  | 40.487 | 1.00 | 36.99 | C |
| ATOM | 578 | O   | ASN | A | 87 | 17.920 | 5.807  | 41.710 | 1.00 | 36.36 | O |
| ATOM | 579 | CB  | ASN | A | 87 | 16.786 | 3.306  | 40.840 | 1.00 | 37.40 | C |
| ATOM | 580 | N   | GLY | A | 88 | 18.676 | 6.224  | 39.618 | 1.00 | 37.00 | N |
| ATOM | 581 | CA  | GLY | A | 88 | 19.593 | 7.272  | 40.056 | 1.00 | 36.90 | C |
| ATOM | 582 | C   | GLY | A | 88 | 18.855 | 8.506  | 40.541 | 1.00 | 36.61 | C |
| ATOM | 583 | O   | GLY | A | 88 | 17.673 | 8.648  | 40.298 | 1.00 | 36.55 | O |
| ATOM | 584 | N   | ASP | A | 89 | 19.532 | 9.392  | 41.250 | 1.00 | 37.05 | N |
| ATOM | 585 | CA  | ASP | A | 89 | 18.882 | 10.640 | 41.687 | 1.00 | 37.92 | C |
| ATOM | 586 | C   | ASP | A | 89 | 18.812 | 11.654 | 40.548 | 1.00 | 37.52 | C |
| ATOM | 587 | O   | ASP | A | 89 | 19.724 | 11.713 | 39.730 | 1.00 | 37.73 | O |
| ATOM | 588 | CB  | ASP | A | 89 | 19.639 | 11.281 | 42.840 | 1.00 | 38.02 | C |
| ATOM | 589 | CG  | ASP | A | 89 | 19.342 | 10.639 | 44.165 | 1.00 | 40.19 | C |
| ATOM | 590 | OD1 | ASP | A | 89 | 18.398 | 9.813  | 44.252 | 1.00 | 44.15 | O |
| ATOM | 591 | OD2 | ASP | A | 89 | 20.002 | 10.918 | 45.186 | 1.00 | 42.25 | O |
| ATOM | 592 | N   | PHE | A | 90 | 17.734 | 12.438 | 40.491 | 1.00 | 37.19 | N |
| ATOM | 593 | CA  | PHE | A | 90 | 17.638 | 13.546 | 39.520 | 1.00 | 36.65 | C |
| ATOM | 594 | C   | PHE | A | 90 | 17.435 | 14.912 | 40.182 | 1.00 | 36.57 | C |
| ATOM | 595 | O   | PHE | A | 90 | 16.551 | 15.078 | 41.015 | 1.00 | 36.80 | O |
| ATOM | 596 | CB  | PHE | A | 90 | 16.512 | 13.310 | 38.516 | 1.00 | 35.79 | C |
| ATOM | 597 | CG  | PHE | A | 90 | 16.793 | 12.200 | 37.551 | 1.00 | 35.34 | C |
| ATOM | 598 | CD1 | PHE | A | 90 | 16.627 | 10.870 | 37.931 | 1.00 | 34.10 | C |
| ATOM | 599 | CD2 | PHE | A | 90 | 17.235 | 12.472 | 36.275 | 1.00 | 34.19 | C |
| ATOM | 600 | CE1 | PHE | A | 90 | 16.875 | 9.854  | 37.061 | 1.00 | 31.47 | C |
| ATOM | 601 | CE2 | PHE | A | 90 | 17.488 | 11.452 | 35.404 | 1.00 | 35.32 | C |
| ATOM | 602 | CZ  | PHE | A | 90 | 17.315 | 10.123 | 35.813 | 1.00 | 34.26 | C |
| ATOM | 603 | N   | SER | A | 91 | 18.257 | 15.886 | 39.803 | 1.00 | 36.85 | N |
| ATOM | 604 | CA  | SER | A | 91 | 18.077 | 17.264 | 40.278 | 1.00 | 37.16 | C |
| ATOM | 605 | C   | SER | A | 91 | 16.856 | 17.884 | 39.612 | 1.00 | 37.28 | C |
| ATOM | 606 | O   | SER | A | 91 | 16.761 | 17.912 | 38.392 | 1.00 | 36.72 | O |
| ATOM | 607 | CB  | SER | A | 91 | 19.278 | 18.146 | 39.971 | 1.00 | 36.75 | C |
| ATOM | 608 | OG  | SER | A | 91 | 20.470 | 17.600 | 40.456 | 1.00 | 35.79 | O |
| ATOM | 609 | N   | VAL | A | 92 | 15.938 | 18.374 | 40.434 | 1.00 | 37.83 | N |
| ATOM | 610 | CA  | VAL | A | 92 | 14.740 | 19.022 | 39.963 | 1.00 | 38.40 | C |
| ATOM | 611 | C   | VAL | A | 92 | 14.549 | 20.334 | 40.690 | 1.00 | 39.41 | C |
| ATOM | 612 | O   | VAL | A | 92 | 14.465 | 20.394 | 41.941 | 1.00 | 39.08 | O |
| ATOM | 613 | CB  | VAL | A | 92 | 13.507 | 18.227 | 40.298 | 1.00 | 38.96 | C |
| ATOM | 614 | CG1 | VAL | A | 92 | 12.270 | 19.005 | 39.893 | 1.00 | 38.57 | C |
| ATOM | 615 | CG2 | VAL | A | 92 | 13.556 | 16.837 | 39.651 | 1.00 | 39.45 | C |
| ATOM | 616 | N   | TYR | A | 93 | 14.426 | 21.386 | 39.895 | 1.00 | 39.95 | N |
| ATOM | 617 | CA  | TYR | A | 93 | 14.214 | 22.701 | 40.419 | 1.00 | 40.34 | C |
| ATOM | 618 | C   | TYR | A | 93 | 12.756 | 22.950 | 40.459 | 1.00 | 40.76 | C |
| ATOM | 619 | O   | TYR | A | 93 | 11.999 | 22.493 | 39.583 | 1.00 | 40.39 | O |
| ATOM | 620 | CB  | TYR | A | 93 | 14.897 | 23.729 | 39.529 | 1.00 | 40.89 | C |
| ATOM | 621 | CG  | TYR | A | 93 | 16.369 | 23.580 | 39.627 | 1.00 | 40.80 | C |
| ATOM | 622 | CD1 | TYR | A | 93 | 17.067 | 24.135 | 40.681 | 1.00 | 40.79 | C |
| ATOM | 623 | CD2 | TYR | A | 93 | 17.042 | 22.801 | 38.743 | 1.00 | 41.05 | C |
| ATOM | 624 | CE1 | TYR | A | 93 | 18.395 | 23.953 | 40.802 | 1.00 | 41.05 | C |
| ATOM | 625 | CE2 | TYR | A | 93 | 18.363 | 22.629 | 38.852 | 1.00 | 42.75 | C |
| ATOM | 626 | CZ  | TYR | A | 93 | 19.037 | 23.204 | 39.881 | 1.00 | 42.45 | C |
| ATOM | 627 | OH  | TYR | A | 93 | 20.372 | 22.965 | 39.971 | 1.00 | 47.63 | O |
| ATOM | 628 | N   | SER | A | 94 | 12.385 | 23.699 | 41.482 | 1.00 | 41.70 | N |
| ATOM | 629 | CA  | SER | A | 94 | 11.014 | 24.053 | 41.743 | 1.00 | 42.70 | C |
| ATOM | 630 | C   | SER | A | 94 | 10.965 | 25.565 | 41.855 | 1.00 | 43.09 | C |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 631 | O   | SER | A | 94  | 11.851 | 26.181 | 42.441 | 1.00 | 43.63 | O |
| ATOM | 632 | CB  | SER | A | 94  | 10.570 | 23.415 | 43.051 | 1.00 | 42.76 | C |
| ATOM | 633 | OG  | SER | A | 94  | 9.258  | 23.841 | 43.395 | 1.00 | 45.05 | O |
| ATOM | 634 | N   | ALA | A | 95  | 9.929  | 26.171 | 41.308 | 1.00 | 43.42 | N |
| ATOM | 635 | CA  | ALA | A | 95  | 9.839  | 27.607 | 41.323 | 1.00 | 43.49 | C |
| ATOM | 636 | C   | ALA | A | 95  | 8.416  | 28.083 | 41.281 | 1.00 | 43.87 | C |
| ATOM | 637 | O   | ALA | A | 95  | 7.520  | 27.416 | 40.789 | 1.00 | 43.95 | O |
| ATOM | 638 | CB  | ALA | A | 95  | 10.572 | 28.164 | 40.145 | 1.00 | 43.70 | C |
| ATOM | 639 | N   | SER | A | 96  | 8.219  | 29.287 | 41.770 | 1.00 | 44.66 | N |
| ATOM | 640 | CA  | SER | A | 96  | 6.901  | 29.866 | 41.757 | 1.00 | 45.08 | C |
| ATOM | 641 | C   | SER | A | 96  | 6.767  | 30.914 | 40.668 | 1.00 | 44.27 | C |
| ATOM | 642 | O   | SER | A | 96  | 5.783  | 31.636 | 40.637 | 1.00 | 45.20 | O |
| ATOM | 643 | CB  | SER | A | 96  | 6.604  | 30.510 | 43.095 | 1.00 | 45.33 | C |
| ATOM | 644 | OG  | SER | A | 96  | 5.384  | 31.199 | 42.973 | 1.00 | 47.96 | O |
| ATOM | 645 | N   | THR | A | 97  | 7.776  | 31.034 | 39.819 | 1.00 | 42.95 | N |
| ATOM | 646 | CA  | THR | A | 97  | 7.738  | 31.962 | 38.688 | 1.00 | 42.08 | C |
| ATOM | 647 | C   | THR | A | 97  | 8.103  | 31.184 | 37.461 | 1.00 | 40.94 | C |
| ATOM | 648 | O   | THR | A | 97  | 8.604  | 30.095 | 37.584 | 1.00 | 40.73 | O |
| ATOM | 649 | CB  | THR | A | 97  | 8.779  | 33.088 | 38.826 | 1.00 | 42.48 | C |
| ATOM | 650 | OG1 | THR | A | 97  | 8.964  | 33.707 | 37.546 | 1.00 | 43.60 | O |
| ATOM | 651 | CG2 | THR | A | 97  | 10.209 | 32.544 | 39.156 | 1.00 | 42.12 | C |
| ATOM | 652 | N   | HIS | A | 98  | 7.904  | 31.734 | 36.275 | 1.00 | 40.18 | N |
| ATOM | 653 | CA  | HIS | A | 98  | 8.319  | 31.012 | 35.074 | 1.00 | 40.09 | C |
| ATOM | 654 | C   | HIS | A | 98  | 9.840  | 31.036 | 34.883 | 1.00 | 39.78 | C |
| ATOM | 655 | O   | HIS | A | 98  | 10.376 | 30.277 | 34.078 | 1.00 | 38.48 | O |
| ATOM | 656 | CB  | HIS | A | 98  | 7.660  | 31.580 | 33.824 | 1.00 | 40.00 | C |
| ATOM | 657 | CG  | HIS | A | 98  | 7.947  | 33.028 | 33.582 | 1.00 | 40.56 | C |
| ATOM | 658 | ND1 | HIS | A | 98  | 7.297  | 34.041 | 34.259 | 1.00 | 40.13 | N |
| ATOM | 659 | CD2 | HIS | A | 98  | 8.805  | 33.640 | 32.729 | 1.00 | 42.26 | C |
| ATOM | 660 | CE1 | HIS | A | 98  | 7.741  | 35.212 | 33.841 | 1.00 | 37.08 | C |
| ATOM | 661 | NE2 | HIS | A | 98  | 8.661  | 35.002 | 32.915 | 1.00 | 39.74 | N |
| ATOM | 662 | N   | LYS | A | 99  | 10.526 | 31.883 | 35.652 | 1.00 | 39.73 | N |
| ATOM | 663 | CA  | LYS | A | 99  | 11.948 | 32.082 | 35.476 | 1.00 | 40.45 | C |
| ATOM | 664 | C   | LYS | A | 99  | 12.861 | 31.221 | 36.332 | 1.00 | 40.34 | C |
| ATOM | 665 | O   | LYS | A | 99  | 12.904 | 31.376 | 37.554 | 1.00 | 41.93 | O |
| ATOM | 666 | CB  | LYS | A | 99  | 12.279 | 33.535 | 35.730 | 1.00 | 40.89 | C |
| ATOM | 667 | CG  | LYS | A | 99  | 11.819 | 34.443 | 34.624 | 1.00 | 43.12 | C |
| ATOM | 668 | CD  | LYS | A | 99  | 12.466 | 35.806 | 34.753 | 1.00 | 46.04 | C |
| ATOM | 669 | CE  | LYS | A | 99  | 11.733 | 36.727 | 35.711 | 1.00 | 48.26 | C |
| ATOM | 670 | NZ  | LYS | A | 99  | 10.662 | 37.495 | 35.003 | 1.00 | 49.55 | N |
| ATOM | 671 | N   | PHE | A | 100 | 13.622 | 30.335 | 35.700 | 1.00 | 39.70 | N |
| ATOM | 672 | CA  | PHE | A | 100 | 14.554 | 29.487 | 36.447 | 1.00 | 39.48 | C |
| ATOM | 673 | C   | PHE | A | 100 | 16.001 | 30.011 | 36.390 | 1.00 | 39.52 | C |
| ATOM | 674 | O   | PHE | A | 100 | 16.874 | 29.435 | 35.718 | 1.00 | 38.87 | O |
| ATOM | 675 | CB  | PHE | A | 100 | 14.485 | 28.056 | 35.939 | 1.00 | 39.33 | C |
| ATOM | 676 | CG  | PHE | A | 100 | 13.266 | 27.328 | 36.377 | 1.00 | 38.47 | C |
| ATOM | 677 | CD1 | PHE | A | 100 | 12.059 | 27.519 | 35.725 | 1.00 | 36.20 | C |
| ATOM | 678 | CD2 | PHE | A | 100 | 13.327 | 26.441 | 37.443 | 1.00 | 37.31 | C |
| ATOM | 679 | CE1 | PHE | A | 100 | 10.960 | 26.846 | 36.125 | 1.00 | 36.52 | C |
| ATOM | 680 | CE2 | PHE | A | 100 | 12.212 | 25.751 | 37.849 | 1.00 | 36.40 | C |
| ATOM | 681 | CZ  | PHE | A | 100 | 11.037 | 25.946 | 37.206 | 1.00 | 36.52 | C |
| ATOM | 682 | N   | LEU | A | 101 | 16.244 | 31.130 | 37.066 | 1.00 | 39.53 | N |
| ATOM | 683 | CA  | LEU | A | 101 | 17.592 | 31.667 | 37.170 | 1.00 | 39.36 | C |
| ATOM | 684 | C   | LEU | A | 101 | 18.548 | 30.642 | 37.787 | 1.00 | 39.88 | C |
| ATOM | 685 | O   | LEU | A | 101 | 18.345 | 30.152 | 38.899 | 1.00 | 39.47 | O |
| ATOM | 686 | CB  | LEU | A | 101 | 17.574 | 32.912 | 38.036 | 1.00 | 39.37 | C |
| ATOM | 687 | CG  | LEU | A | 101 | 18.828 | 33.777 | 38.071 | 1.00 | 39.44 | C |
| ATOM | 688 | CD1 | LEU | A | 101 | 19.258 | 34.290 | 36.693 | 1.00 | 37.56 | C |
| ATOM | 689 | CD2 | LEU | A | 101 | 18.546 | 34.926 | 39.008 | 1.00 | 39.90 | C |
| ATOM | 690 | N   | TYR | A | 102 | 19.578 | 30.297 | 37.032 | 1.00 | 41.10 | N |
| ATOM | 691 | CA  | TYR | A | 102 | 20.623 | 29.415 | 37.507 | 1.00 | 41.59 | C |



|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 692 | C   | TYR | A | 102 | 21.439 | 30.097 | 38.611 | 1.00 | 42.23 | C |
| ATOM | 693 | O   | TYR | A | 102 | 21.778 | 31.296 | 38.500 | 1.00 | 42.28 | O |
| ATOM | 694 | CB  | TYR | A | 102 | 21.580 | 29.048 | 36.370 | 1.00 | 41.49 | C |
| ATOM | 695 | CG  | TYR | A | 102 | 22.706 | 28.209 | 36.894 | 1.00 | 43.02 | C |
| ATOM | 696 | CD1 | TYR | A | 102 | 22.507 | 26.864 | 37.200 | 1.00 | 42.85 | C |
| ATOM | 697 | CD2 | TYR | A | 102 | 23.941 | 28.761 | 37.150 | 1.00 | 43.85 | C |
| ATOM | 698 | CE1 | TYR | A | 102 | 23.504 | 26.110 | 37.725 | 1.00 | 45.04 | C |
| ATOM | 699 | CE2 | TYR | A | 102 | 24.942 | 28.005 | 37.696 | 1.00 | 46.05 | C |
| ATOM | 700 | CZ  | TYR | A | 102 | 24.725 | 26.681 | 37.984 | 1.00 | 46.73 | C |
| ATOM | 701 | OH  | TYR | A | 102 | 25.752 | 25.915 | 38.544 | 1.00 | 52.49 | O |
| ATOM | 702 | N   | TYR | A | 103 | 21.759 | 29.340 | 39.657 | 1.00 | 42.12 | N |
| ATOM | 703 | CA  | TYR | A | 103 | 22.665 | 29.832 | 40.690 | 1.00 | 42.58 | C |
| ATOM | 704 | C   | TYR | A | 103 | 23.632 | 28.750 | 41.207 | 1.00 | 41.98 | C |
| ATOM | 705 | O   | TYR | A | 103 | 23.333 | 27.560 | 41.237 | 1.00 | 42.05 | O |
| ATOM | 706 | CB  | TYR | A | 103 | 21.901 | 30.435 | 41.843 | 1.00 | 43.03 | C |
| ATOM | 707 | CG  | TYR | A | 103 | 20.964 | 29.493 | 42.477 | 1.00 | 44.79 | C |
| ATOM | 708 | CD1 | TYR | A | 103 | 19.691 | 29.333 | 41.971 | 1.00 | 47.69 | C |
| ATOM | 709 | CD2 | TYR | A | 103 | 21.338 | 28.769 | 43.590 | 1.00 | 49.51 | C |
| ATOM | 710 | CE1 | TYR | A | 103 | 18.798 | 28.456 | 42.544 | 1.00 | 50.63 | C |
| ATOM | 711 | CE2 | TYR | A | 103 | 20.449 | 27.890 | 44.202 | 1.00 | 52.43 | C |
| ATOM | 712 | CZ  | TYR | A | 103 | 19.181 | 27.736 | 43.658 | 1.00 | 52.68 | C |
| ATOM | 713 | OH  | TYR | A | 103 | 18.297 | 26.875 | 44.234 | 1.00 | 56.40 | O |
| ATOM | 714 | N   | ASP | A | 104 | 24.809 | 29.190 | 41.603 | 1.00 | 41.00 | N |
| ATOM | 715 | CA  | ASP | A | 104 | 25.844 | 28.288 | 42.026 | 1.00 | 40.33 | C |
| ATOM | 716 | C   | ASP | A | 104 | 25.842 | 28.250 | 43.530 | 1.00 | 39.98 | C |
| ATOM | 717 | O   | ASP | A | 104 | 26.177 | 29.224 | 44.219 | 1.00 | 38.58 | O |
| ATOM | 718 | CB  | ASP | A | 104 | 27.169 | 28.768 | 41.492 | 1.00 | 40.13 | C |
| ATOM | 719 | CG  | ASP | A | 104 | 28.310 | 27.929 | 41.958 | 1.00 | 42.26 | C |
| ATOM | 720 | OD1 | ASP | A | 104 | 28.117 | 27.151 | 42.942 | 1.00 | 44.33 | O |
| ATOM | 721 | OD2 | ASP | A | 104 | 29.429 | 27.989 | 41.393 | 1.00 | 42.30 | O |
| ATOM | 722 | N   | GLU | A | 105 | 25.425 | 27.110 | 44.041 | 1.00 | 40.20 | N |
| ATOM | 723 | CA  | GLU | A | 105 | 25.294 | 26.950 | 45.472 | 1.00 | 40.26 | C |
| ATOM | 724 | C   | GLU | A | 105 | 26.605 | 27.213 | 46.228 | 1.00 | 39.92 | C |
| ATOM | 725 | O   | GLU | A | 105 | 26.577 | 27.824 | 47.293 | 1.00 | 40.11 | O |
| ATOM | 726 | CB  | GLU | A | 105 | 24.747 | 25.570 | 45.744 | 1.00 | 40.54 | C |
| ATOM | 727 | CG  | GLU | A | 105 | 23.245 | 25.502 | 45.533 | 1.00 | 42.55 | C |
| ATOM | 728 | CD  | GLU | A | 105 | 22.709 | 24.086 | 45.506 | 1.00 | 44.11 | C |
| ATOM | 729 | OE1 | GLU | A | 105 | 23.178 | 23.251 | 46.323 | 1.00 | 46.78 | O |
| ATOM | 730 | OE2 | GLU | A | 105 | 21.801 | 23.815 | 44.684 | 1.00 | 42.74 | O |
| ATOM | 731 | N   | LYS | A | 106 | 27.748 | 26.819 | 45.661 | 1.00 | 39.52 | N |
| ATOM | 732 | CA  | LYS | A | 106 | 29.041 | 26.991 | 46.336 | 1.00 | 39.53 | C |
| ATOM | 733 | C   | LYS | A | 106 | 29.370 | 28.419 | 46.623 | 1.00 | 39.68 | C |
| ATOM | 734 | O   | LYS | A | 106 | 30.199 | 28.697 | 47.471 | 1.00 | 40.24 | O |
| ATOM | 735 | CB  | LYS | A | 106 | 30.221 | 26.479 | 45.504 | 1.00 | 39.89 | C |
| ATOM | 736 | CG  | LYS | A | 106 | 30.257 | 24.976 | 45.143 | 1.00 | 40.25 | C |
| ATOM | 737 | N   | LYS | A | 107 | 28.747 | 29.333 | 45.894 | 1.00 | 40.07 | N |
| ATOM | 738 | CA  | LYS | A | 107 | 29.043 | 30.740 | 46.031 | 1.00 | 39.35 | C |
| ATOM | 739 | C   | LYS | A | 107 | 28.061 | 31.421 | 46.937 | 1.00 | 39.82 | C |
| ATOM | 740 | O   | LYS | A | 107 | 28.208 | 32.586 | 47.188 | 1.00 | 39.28 | O |
| ATOM | 741 | CB  | LYS | A | 107 | 29.050 | 31.410 | 44.645 | 1.00 | 39.29 | C |
| ATOM | 742 | CG  | LYS | A | 107 | 30.329 | 31.155 | 43.827 | 1.00 | 37.47 | C |
| ATOM | 743 | CD  | LYS | A | 107 | 30.286 | 31.702 | 42.406 | 1.00 | 34.55 | C |
| ATOM | 744 | CE  | LYS | A | 107 | 31.606 | 31.470 | 41.651 | 1.00 | 33.57 | C |
| ATOM | 745 | NZ  | LYS | A | 107 | 31.607 | 31.880 | 40.178 | 1.00 | 30.95 | N |
| ATOM | 746 | N   | MET | A | 108 | 27.071 | 30.707 | 47.458 | 1.00 | 41.78 | N |
| ATOM | 747 | CA  | MET | A | 108 | 26.079 | 31.341 | 48.341 | 1.00 | 43.69 | C |
| ATOM | 748 | C   | MET | A | 108 | 26.621 | 31.950 | 49.646 | 1.00 | 44.68 | C |
| ATOM | 749 | O   | MET | A | 108 | 26.154 | 33.004 | 50.061 | 1.00 | 44.99 | O |
| ATOM | 750 | CB  | MET | A | 108 | 24.923 | 30.396 | 48.594 | 1.00 | 44.05 | C |
| ATOM | 751 | CG  | MET | A | 108 | 24.195 | 30.105 | 47.282 | 1.00 | 46.49 | C |
| ATOM | 752 | SD  | MET | A | 108 | 22.723 | 29.125 | 47.315 | 1.00 | 51.54 | S |



|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 753 | CE  | MET | A | 108 | 21.653 | 30.080 | 48.484 | 1.00 | 51.43 | C |
| ATOM | 754 | N   | ALA | A | 109 | 27.630 | 31.341 | 50.254 | 1.00 | 46.34 | N |
| ATOM | 755 | CA  | ALA | A | 109 | 28.211 | 31.855 | 51.510 | 1.00 | 47.87 | C |
| ATOM | 756 | C   | ALA | A | 109 | 28.697 | 33.308 | 51.406 | 1.00 | 49.27 | C |
| ATOM | 757 | O   | ALA | A | 109 | 28.533 | 34.114 | 52.323 | 1.00 | 49.44 | O |
| ATOM | 758 | CB  | ALA | A | 109 | 29.355 | 30.958 | 51.960 | 1.00 | 47.63 | C |
| ATOM | 759 | N   | ASN | A | 110 | 29.276 | 33.651 | 50.269 | 1.00 | 50.88 | N |
| ATOM | 760 | CA  | ASN | A | 110 | 29.792 | 35.004 | 50.069 | 1.00 | 51.99 | C |
| ATOM | 761 | C   | ASN | A | 110 | 28.732 | 36.070 | 49.736 | 1.00 | 51.88 | C |
| ATOM | 762 | O   | ASN | A | 110 | 29.038 | 37.252 | 49.562 | 1.00 | 51.14 | O |
| ATOM | 763 | CB  | ASN | A | 110 | 30.876 | 34.939 | 48.994 | 1.00 | 52.43 | C |
| ATOM | 764 | CG  | ASN | A | 110 | 32.077 | 34.080 | 49.433 | 1.00 | 54.41 | C |
| ATOM | 765 | OD1 | ASN | A | 110 | 32.460 | 34.050 | 50.624 | 1.00 | 54.72 | O |
| ATOM | 766 | ND2 | ASN | A | 110 | 32.663 | 33.373 | 48.478 | 1.00 | 56.75 | N |
| ATOM | 767 | N   | PHE | A | 111 | 27.484 | 35.651 | 49.632 | 1.00 | 52.59 | N |
| ATOM | 768 | CA  | PHE | A | 111 | 26.404 | 36.598 | 49.409 | 1.00 | 53.32 | C |
| ATOM | 769 | C   | PHE | A | 111 | 25.202 | 36.180 | 50.261 | 1.00 | 54.75 | C |
| ATOM | 770 | O   | PHE | A | 111 | 24.149 | 35.801 | 49.749 | 1.00 | 54.37 | O |
| ATOM | 771 | CB  | PHE | A | 111 | 26.053 | 36.693 | 47.923 | 1.00 | 52.83 | C |
| ATOM | 772 | CG  | PHE | A | 111 | 27.058 | 37.461 | 47.107 | 1.00 | 50.42 | C |
| ATOM | 773 | CD1 | PHE | A | 111 | 28.283 | 36.907 | 46.791 | 1.00 | 49.93 | C |
| ATOM | 774 | CD2 | PHE | A | 111 | 26.781 | 38.729 | 46.658 | 1.00 | 48.60 | C |
| ATOM | 775 | CE1 | PHE | A | 111 | 29.205 | 37.609 | 46.044 | 1.00 | 49.18 | C |
| ATOM | 776 | CE2 | PHE | A | 111 | 27.701 | 39.429 | 45.904 | 1.00 | 47.91 | C |
| ATOM | 777 | CZ  | PHE | A | 111 | 28.910 | 38.869 | 45.601 | 1.00 | 47.42 | C |
| ATOM | 778 | N   | GLN | A | 112 | 25.376 | 36.279 | 51.576 | 1.00 | 56.74 | N |
| ATOM | 779 | CA  | GLN | A | 112 | 24.353 | 35.855 | 52.536 | 1.00 | 58.14 | C |
| ATOM | 780 | C   | GLN | A | 112 | 22.970 | 36.399 | 52.192 | 1.00 | 58.29 | C |
| ATOM | 781 | O   | GLN | A | 112 | 21.972 | 35.742 | 52.468 | 1.00 | 58.53 | O |
| ATOM | 782 | CB  | GLN | A | 112 | 24.730 | 36.282 | 53.961 | 1.00 | 58.65 | C |
| ATOM | 783 | CG  | GLN | A | 112 | 26.100 | 35.815 | 54.441 | 1.00 | 61.33 | C |
| ATOM | 784 | CD  | GLN | A | 112 | 26.213 | 34.307 | 54.467 | 1.00 | 64.34 | C |
| ATOM | 785 | OE1 | GLN | A | 112 | 25.483 | 33.622 | 53.750 | 1.00 | 66.46 | O |
| ATOM | 786 | NE2 | GLN | A | 112 | 27.133 | 33.784 | 55.281 | 1.00 | 66.00 | N |
| ATOM | 787 | N   | ASN | A | 113 | 22.919 | 37.581 | 51.580 | 1.00 | 58.45 | N |
| ATOM | 788 | CA  | ASN | A | 113 | 21.653 | 38.222 | 51.240 | 1.00 | 58.79 | C |
| ATOM | 789 | C   | ASN | A | 113 | 21.000 | 37.740 | 49.936 | 1.00 | 58.82 | C |
| ATOM | 790 | O   | ASN | A | 113 | 19.971 | 38.284 | 49.536 | 1.00 | 59.69 | O |
| ATOM | 791 | CB  | ASN | A | 113 | 21.813 | 39.759 | 51.171 | 1.00 | 58.81 | C |
| ATOM | 792 | CG  | ASN | A | 113 | 22.160 | 40.387 | 52.525 | 1.00 | 59.17 | C |
| ATOM | 793 | OD1 | ASN | A | 113 | 21.863 | 39.824 | 53.593 | 1.00 | 57.49 | O |
| ATOM | 794 | ND2 | ASN | A | 113 | 22.786 | 41.567 | 52.482 | 1.00 | 58.34 | N |
| ATOM | 795 | N   | PHE | A | 114 | 21.570 | 36.760 | 49.245 | 1.00 | 58.33 | N |
| ATOM | 796 | CA  | PHE | A | 114 | 20.930 | 36.306 | 48.015 | 1.00 | 57.84 | C |
| ATOM | 797 | C   | PHE | A | 114 | 19.922 | 35.220 | 48.334 | 1.00 | 57.57 | C |
| ATOM | 798 | O   | PHE | A | 114 | 20.264 | 34.208 | 48.953 | 1.00 | 57.24 | O |
| ATOM | 799 | CB  | PHE | A | 114 | 21.933 | 35.774 | 47.013 | 1.00 | 57.99 | C |
| ATOM | 800 | CG  | PHE | A | 114 | 21.289 | 35.126 | 45.822 | 1.00 | 58.28 | C |
| ATOM | 801 | CD1 | PHE | A | 114 | 20.642 | 35.897 | 44.867 | 1.00 | 58.11 | C |
| ATOM | 802 | CD2 | PHE | A | 114 | 21.300 | 33.744 | 45.674 | 1.00 | 58.56 | C |
| ATOM | 803 | CE1 | PHE | A | 114 | 20.028 | 35.312 | 43.781 | 1.00 | 58.29 | C |
| ATOM | 804 | CE2 | PHE | A | 114 | 20.687 | 33.149 | 44.580 | 1.00 | 59.09 | C |
| ATOM | 805 | CZ  | PHE | A | 114 | 20.050 | 33.937 | 43.630 | 1.00 | 58.80 | C |
| ATOM | 806 | N   | LYS | A | 115 | 18.686 | 35.429 | 47.899 | 1.00 | 57.18 | N |
| ATOM | 807 | CA  | LYS | A | 115 | 17.604 | 34.511 | 48.204 | 1.00 | 57.19 | C |
| ATOM | 808 | C   | LYS | A | 115 | 17.037 | 33.942 | 46.903 | 1.00 | 57.17 | C |
| ATOM | 809 | O   | LYS | A | 115 | 16.268 | 34.598 | 46.193 | 1.00 | 57.12 | O |
| ATOM | 810 | CB  | LYS | A | 115 | 16.524 | 35.234 | 49.016 | 1.00 | 57.33 | C |
| ATOM | 811 | N   | PRO | A | 116 | 17.384 | 32.699 | 46.610 | 1.00 | 56.97 | N |
| ATOM | 812 | CA  | PRO | A | 116 | 17.042 | 32.097 | 45.319 | 1.00 | 57.01 | C |
| ATOM | 813 | C   | PRO | A | 116 | 15.554 | 31.979 | 45.151 | 1.00 | 56.69 | C |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 814 | O   | PRO | A | 116 | 14.864 | 31.676 | 46.103 | 1.00 | 57.03 | O |
| ATOM | 815 | CB  | PRO | A | 116 | 17.672 | 30.701 | 45.378 | 1.00 | 57.15 | C |
| ATOM | 816 | CG  | PRO | A | 116 | 18.474 | 30.658 | 46.662 | 1.00 | 57.53 | C |
| ATOM | 817 | CD  | PRO | A | 116 | 18.045 | 31.763 | 47.522 | 1.00 | 57.03 | C |
| ATOM | 818 | N   | ARG | A | 117 | 15.073 | 32.212 | 43.945 | 1.00 | 56.65 | N |
| ATOM | 819 | CA  | ARG | A | 117 | 13.663 | 32.087 | 43.656 | 1.00 | 56.39 | C |
| ATOM | 820 | C   | ARG | A | 117 | 13.335 | 30.639 | 43.332 | 1.00 | 56.16 | C |
| ATOM | 821 | O   | ARG | A | 117 | 12.160 | 30.272 | 43.279 | 1.00 | 56.65 | O |
| ATOM | 822 | CB  | ARG | A | 117 | 13.280 | 32.971 | 42.508 | 1.00 | 56.56 | C |
| ATOM | 823 | N   | SER | A | 118 | 14.350 | 29.810 | 43.110 | 1.00 | 55.25 | N |
| ATOM | 824 | CA  | SER | A | 118 | 14.083 | 28.393 | 42.878 | 1.00 | 55.12 | C |
| ATOM | 825 | C   | SER | A | 118 | 14.924 | 27.511 | 43.809 | 1.00 | 54.45 | C |
| ATOM | 826 | O   | SER | A | 118 | 16.022 | 27.895 | 44.174 | 1.00 | 54.64 | O |
| ATOM | 827 | CB  | SER | A | 118 | 14.322 | 28.029 | 41.415 | 1.00 | 54.89 | C |
| ATOM | 828 | OG  | SER | A | 118 | 15.672 | 28.196 | 41.087 | 1.00 | 55.13 | O |
| ATOM | 829 | N   | ASN | A | 119 | 14.381 | 26.362 | 44.211 | 1.00 | 53.66 | N |
| ATOM | 830 | CA  | ASN | A | 119 | 15.089 | 25.412 | 45.060 | 1.00 | 53.43 | C |
| ATOM | 831 | C   | ASN | A | 119 | 15.307 | 24.118 | 44.326 | 1.00 | 51.73 | C |
| ATOM | 832 | O   | ASN | A | 119 | 14.472 | 23.705 | 43.552 | 1.00 | 51.23 | O |
| ATOM | 833 | CB  | ASN | A | 119 | 14.277 | 25.063 | 46.311 | 1.00 | 54.32 | C |
| ATOM | 834 | CG  | ASN | A | 119 | 13.711 | 26.272 | 46.994 | 1.00 | 57.18 | C |
| ATOM | 835 | OD1 | ASN | A | 119 | 14.448 | 27.099 | 47.563 | 1.00 | 60.84 | O |
| ATOM | 836 | ND2 | ASN | A | 119 | 12.384 | 26.384 | 46.964 | 1.00 | 61.01 | N |
| ATOM | 837 | N   | ARG | A | 120 | 16.418 | 23.470 | 44.621 | 1.00 | 50.77 | N |
| ATOM | 838 | CA  | ARG | A | 120 | 16.772 | 22.182 | 44.049 | 1.00 | 49.89 | C |
| ATOM | 839 | C   | ARG | A | 120 | 16.388 | 21.062 | 44.999 | 1.00 | 49.87 | C |
| ATOM | 840 | O   | ARG | A | 120 | 16.620 | 21.150 | 46.206 | 1.00 | 50.40 | O |
| ATOM | 841 | CB  | ARG | A | 120 | 18.283 | 22.133 | 43.843 | 1.00 | 49.75 | C |
| ATOM | 842 | CG  | ARG | A | 120 | 18.799 | 20.901 | 43.144 | 1.00 | 47.86 | C |
| ATOM | 843 | CD  | ARG | A | 120 | 20.318 | 20.812 | 43.074 | 1.00 | 45.29 | C |
| ATOM | 844 | NE  | ARG | A | 120 | 20.972 | 21.240 | 44.301 | 1.00 | 43.79 | N |
| ATOM | 845 | CZ  | ARG | A | 120 | 21.316 | 20.432 | 45.314 | 1.00 | 43.05 | C |
| ATOM | 846 | NH1 | ARG | A | 120 | 21.053 | 19.126 | 45.277 | 1.00 | 40.07 | N |
| ATOM | 847 | NH2 | ARG | A | 120 | 21.921 | 20.942 | 46.379 | 1.00 | 41.03 | N |
| ATOM | 848 | N   | GLU | A | 121 | 15.801 | 20.010 | 44.451 | 1.00 | 49.51 | N |
| ATOM | 849 | CA  | GLU | A | 121 | 15.435 | 18.830 | 45.206 | 1.00 | 48.90 | C |
| ATOM | 850 | C   | GLU | A | 121 | 15.905 | 17.609 | 44.411 | 1.00 | 47.95 | C |
| ATOM | 851 | O   | GLU | A | 121 | 15.793 | 17.564 | 43.192 | 1.00 | 48.02 | O |
| ATOM | 852 | CB  | GLU | A | 121 | 13.922 | 18.782 | 45.461 | 1.00 | 49.38 | C |
| ATOM | 853 | CG  | GLU | A | 121 | 13.444 | 17.500 | 46.141 | 1.00 | 51.77 | C |
| ATOM | 854 | CD  | GLU | A | 121 | 12.185 | 17.695 | 46.961 | 1.00 | 54.65 | C |
| ATOM | 855 | OE1 | GLU | A | 121 | 12.312 | 18.258 | 48.073 | 1.00 | 58.68 | O |
| ATOM | 856 | OE2 | GLU | A | 121 | 11.087 | 17.284 | 46.512 | 1.00 | 55.59 | O |
| ATOM | 857 | N   | GLU | A | 122 | 16.455 | 16.622 | 45.104 | 1.00 | 47.05 | N |
| ATOM | 858 | CA  | GLU | A | 122 | 16.938 | 15.423 | 44.463 | 1.00 | 46.05 | C |
| ATOM | 859 | C   | GLU | A | 122 | 15.848 | 14.400 | 44.594 | 1.00 | 45.48 | C |
| ATOM | 860 | O   | GLU | A | 122 | 15.313 | 14.220 | 45.666 | 1.00 | 45.63 | O |
| ATOM | 861 | CB  | GLU | A | 122 | 18.200 | 14.940 | 45.158 | 1.00 | 45.67 | C |
| ATOM | 862 | CG  | GLU | A | 122 | 19.346 | 15.921 | 45.063 | 1.00 | 44.97 | C |
| ATOM | 863 | CD  | GLU | A | 122 | 19.789 | 16.154 | 43.623 | 1.00 | 45.49 | C |
| ATOM | 864 | OE1 | GLU | A | 122 | 19.985 | 15.144 | 42.902 | 1.00 | 44.79 | O |
| ATOM | 865 | OE2 | GLU | A | 122 | 19.925 | 17.337 | 43.207 | 1.00 | 42.47 | O |
| ATOM | 866 | N   | MET | A | 123 | 15.481 | 13.751 | 43.503 | 1.00 | 44.95 | N |
| ATOM | 867 | CA  | MET | A | 123 | 14.462 | 12.731 | 43.589 | 1.00 | 44.35 | C |
| ATOM | 868 | C   | MET | A | 123 | 14.657 | 11.712 | 42.503 | 1.00 | 43.59 | C |
| ATOM | 869 | O   | MET | A | 123 | 15.495 | 11.891 | 41.613 | 1.00 | 43.44 | O |
| ATOM | 870 | CB  | MET | A | 123 | 13.078 | 13.358 | 43.490 | 1.00 | 44.59 | C |
| ATOM | 871 | CG  | MET | A | 123 | 12.831 | 14.092 | 42.205 | 1.00 | 45.95 | C |
| ATOM | 872 | SD  | MET | A | 123 | 11.244 | 14.946 | 42.206 | 1.00 | 47.99 | S |
| ATOM | 873 | CE  | MET | A | 123 | 11.648 | 16.411 | 43.089 | 1.00 | 47.81 | C |
| ATOM | 874 | N   | LYS | A | 124 | 13.880 | 10.638 | 42.603 | 1.00 | 42.37 | N |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 875 | CA  | LYS | A | 124 | 13.869 | 9.575  | 41.623 | 1.00 | 41.47 | C |
| ATOM | 876 | C   | LYS | A | 124 | 12.958 | 10.026 | 40.469 | 1.00 | 40.66 | C |
| ATOM | 877 | O   | LYS | A | 124 | 12.066 | 10.862 | 40.654 | 1.00 | 39.80 | O |
| ATOM | 878 | CB  | LYS | A | 124 | 13.354 | 8.267  | 42.250 | 1.00 | 41.45 | C |
| ATOM | 879 | CG  | LYS | A | 124 | 14.160 | 7.756  | 43.470 | 1.00 | 41.70 | C |
| ATOM | 880 | CD  | LYS | A | 124 | 15.574 | 7.301  | 43.076 | 1.00 | 42.20 | C |
| ATOM | 881 | CE  | LYS | A | 124 | 16.451 | 6.989  | 44.273 | 1.00 | 41.37 | C |
| ATOM | 882 | NZ  | LYS | A | 124 | 17.894 | 7.201  | 43.966 | 1.00 | 41.63 | N |
| ATOM | 883 | N   | PHE | A | 125 | 13.178 | 9.460  | 39.284 | 1.00 | 39.69 | N |
| ATOM | 884 | CA  | PHE | A | 125 | 12.463 | 9.889  | 38.101 | 1.00 | 38.95 | C |
| ATOM | 885 | C   | PHE | A | 125 | 10.981 | 9.729  | 38.257 | 1.00 | 38.85 | C |
| ATOM | 886 | O   | PHE | A | 125 | 10.217 | 10.613 | 37.890 | 1.00 | 37.81 | O |
| ATOM | 887 | CB  | PHE | A | 125 | 12.942 | 9.154  | 36.862 | 1.00 | 38.45 | C |
| ATOM | 888 | CG  | PHE | A | 125 | 12.618 | 9.871  | 35.610 | 1.00 | 39.49 | C |
| ATOM | 889 | CD1 | PHE | A | 125 | 13.471 | 10.840 | 35.118 | 1.00 | 40.78 | C |
| ATOM | 890 | CD2 | PHE | A | 125 | 11.428 | 9.655  | 34.967 | 1.00 | 40.81 | C |
| ATOM | 891 | CE1 | PHE | A | 125 | 13.181 | 11.530 | 33.992 | 1.00 | 40.48 | C |
| ATOM | 892 | CE2 | PHE | A | 125 | 11.123 | 10.353 | 33.825 | 1.00 | 41.39 | C |
| ATOM | 893 | CZ  | PHE | A | 125 | 12.008 | 11.300 | 33.335 | 1.00 | 41.11 | C |
| ATOM | 894 | N   | HIS | A | 126 | 10.575 | 8.602  | 38.835 | 1.00 | 39.49 | N |
| ATOM | 895 | CA  | HIS | A | 126 | 9.161  | 8.342  | 39.044 | 1.00 | 39.91 | C |
| ATOM | 896 | C   | HIS | A | 126 | 8.599  | 9.408  | 39.976 | 1.00 | 39.98 | C |
| ATOM | 897 | O   | HIS | A | 126 | 7.455  | 9.821  | 39.830 | 1.00 | 39.26 | O |
| ATOM | 898 | CB  | HIS | A | 126 | 8.906  | 6.899  | 39.552 | 1.00 | 40.45 | C |
| ATOM | 899 | CG  | HIS | A | 126 | 9.034  | 6.727  | 41.033 | 1.00 | 41.06 | C |
| ATOM | 900 | ND1 | HIS | A | 126 | 7.987  | 6.950  | 41.899 | 1.00 | 40.98 | N |
| ATOM | 901 | CD2 | HIS | A | 126 | 10.092 | 6.367  | 41.801 | 1.00 | 41.92 | C |
| ATOM | 902 | CE1 | HIS | A | 126 | 8.403  | 6.759  | 43.140 | 1.00 | 43.22 | C |
| ATOM | 903 | NE2 | HIS | A | 126 | 9.676  | 6.405  | 43.108 | 1.00 | 42.45 | N |
| ATOM | 904 | N   | GLU | A | 127 | 9.428  | 9.898  | 40.890 | 1.00 | 40.59 | N |
| ATOM | 905 | CA  | GLU | A | 127 | 8.975  | 10.919 | 41.824 | 1.00 | 41.56 | C |
| ATOM | 906 | C   | GLU | A | 127 | 8.749  | 12.213 | 41.062 | 1.00 | 41.66 | C |
| ATOM | 907 | O   | GLU | A | 127 | 7.774  | 12.941 | 41.294 | 1.00 | 41.64 | O |
| ATOM | 908 | CB  | GLU | A | 127 | 9.968  | 11.102 | 42.978 | 1.00 | 41.64 | C |
| ATOM | 909 | CG  | GLU | A | 127 | 10.149 | 9.839  | 43.811 | 1.00 | 43.10 | C |
| ATOM | 910 | CD  | GLU | A | 127 | 11.116 | 10.017 | 44.958 | 1.00 | 44.79 | C |
| ATOM | 911 | OE1 | GLU | A | 127 | 12.326 | 10.217 | 44.712 | 1.00 | 43.71 | O |
| ATOM | 912 | OE2 | GLU | A | 127 | 10.649 | 9.938  | 46.122 | 1.00 | 49.43 | O |
| ATOM | 913 | N   | PHE | A | 128 | 9.636  | 12.491 | 40.124 | 1.00 | 41.96 | N |
| ATOM | 914 | CA  | PHE | A | 128 | 9.504  | 13.705 | 39.337 | 1.00 | 41.99 | C |
| ATOM | 915 | C   | PHE | A | 128 | 8.213  | 13.612 | 38.538 | 1.00 | 42.56 | C |
| ATOM | 916 | O   | PHE | A | 128 | 7.400  | 14.537 | 38.507 | 1.00 | 41.93 | O |
| ATOM | 917 | CB  | PHE | A | 128 | 10.708 | 13.864 | 38.416 | 1.00 | 41.57 | C |
| ATOM | 918 | CG  | PHE | A | 128 | 10.470 | 14.795 | 37.244 | 1.00 | 41.38 | C |
| ATOM | 919 | CD1 | PHE | A | 128 | 10.199 | 16.136 | 37.449 | 1.00 | 39.65 | C |
| ATOM | 920 | CD2 | PHE | A | 128 | 10.537 | 14.330 | 35.950 | 1.00 | 39.22 | C |
| ATOM | 921 | CE1 | PHE | A | 128 | 9.980  | 16.975 | 36.399 | 1.00 | 40.36 | C |
| ATOM | 922 | CE2 | PHE | A | 128 | 10.329 | 15.191 | 34.888 | 1.00 | 41.57 | C |
| ATOM | 923 | CZ  | PHE | A | 128 | 10.044 | 16.510 | 35.112 | 1.00 | 40.14 | C |
| ATOM | 924 | N   | VAL | A | 129 | 7.999  | 12.463 | 37.921 | 1.00 | 43.85 | N |
| ATOM | 925 | CA  | VAL | A | 129 | 6.813  | 12.288 | 37.095 | 1.00 | 44.87 | C |
| ATOM | 926 | C   | VAL | A | 129 | 5.536  | 12.443 | 37.932 | 1.00 | 46.07 | C |
| ATOM | 927 | O   | VAL | A | 129 | 4.574  | 13.093 | 37.505 | 1.00 | 45.32 | O |
| ATOM | 928 | CB  | VAL | A | 129 | 6.798  | 10.920 | 36.425 | 1.00 | 44.99 | C |
| ATOM | 929 | CG1 | VAL | A | 129 | 5.496  | 10.725 | 35.631 | 1.00 | 44.81 | C |
| ATOM | 930 | CG2 | VAL | A | 129 | 8.030  | 10.718 | 35.550 | 1.00 | 43.96 | C |
| ATOM | 931 | N   | GLU | A | 130 | 5.553  | 11.854 | 39.128 | 1.00 | 47.64 | N |
| ATOM | 932 | CA  | GLU | A | 130 | 4.415  | 11.932 | 40.037 | 1.00 | 49.12 | C |
| ATOM | 933 | C   | GLU | A | 130 | 4.136  | 13.390 | 40.384 | 1.00 | 49.48 | C |
| ATOM | 934 | O   | GLU | A | 130 | 3.003  | 13.846 | 40.250 | 1.00 | 48.66 | O |
| ATOM | 935 | CB  | GLU | A | 130 | 4.654  | 11.079 | 41.296 | 1.00 | 49.63 | C |



|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 936 | CG  | GLU | A | 130 | 4.534  | 9.576  | 41.062 | 1.00 | 50.81 | C |
| ATOM | 937 | CD  | GLU | A | 130 | 5.257  | 8.747  | 42.117 | 1.00 | 53.77 | C |
| ATOM | 938 | OE1 | GLU | A | 130 | 5.566  | 9.295  | 43.204 | 1.00 | 55.27 | O |
| ATOM | 939 | OE2 | GLU | A | 130 | 5.518  | 7.543  | 41.856 | 1.00 | 54.73 | O |
| ATOM | 940 | N   | LYS | A | 131 | 5.170  | 14.121 | 40.798 | 1.00 | 50.56 | N |
| ATOM | 941 | CA  | LYS | A | 131 | 5.010  | 15.547 | 41.082 | 1.00 | 51.84 | C |
| ATOM | 942 | C   | LYS | A | 131 | 4.385  | 16.276 | 39.886 | 1.00 | 52.55 | C |
| ATOM | 943 | O   | LYS | A | 131 | 3.482  | 17.070 | 40.061 | 1.00 | 52.15 | O |
| ATOM | 944 | CB  | LYS | A | 131 | 6.340  | 16.209 | 41.438 | 1.00 | 52.23 | C |
| ATOM | 945 | CG  | LYS | A | 131 | 6.554  | 16.568 | 42.907 | 1.00 | 53.75 | C |
| ATOM | 946 | CD  | LYS | A | 131 | 7.249  | 17.944 | 43.054 | 1.00 | 56.27 | C |
| ATOM | 947 | CE  | LYS | A | 131 | 7.879  | 18.168 | 44.448 | 1.00 | 58.66 | C |
| ATOM | 948 | NZ  | LYS | A | 131 | 8.247  | 19.628 | 44.725 | 1.00 | 59.31 | N |
| ATOM | 949 | N   | LEU | A | 132 | 4.845  | 16.014 | 38.667 | 1.00 | 53.84 | N |
| ATOM | 950 | CA  | LEU | A | 132 | 4.247  | 16.691 | 37.513 | 1.00 | 55.23 | C |
| ATOM | 951 | C   | LEU | A | 132 | 2.762  | 16.408 | 37.407 | 1.00 | 55.96 | C |
| ATOM | 952 | O   | LEU | A | 132 | 1.973  | 17.292 | 37.063 | 1.00 | 55.69 | O |
| ATOM | 953 | CB  | LEU | A | 132 | 4.906  | 16.278 | 36.206 | 1.00 | 55.45 | C |
| ATOM | 954 | CG  | LEU | A | 132 | 6.301  | 16.811 | 35.966 | 1.00 | 56.60 | C |
| ATOM | 955 | CD1 | LEU | A | 132 | 6.785  | 16.291 | 34.646 | 1.00 | 57.60 | C |
| ATOM | 956 | CD2 | LEU | A | 132 | 6.303  | 18.327 | 35.966 | 1.00 | 57.89 | C |
| ATOM | 957 | N   | GLN | A | 133 | 2.397  | 15.157 | 37.669 | 1.00 | 57.19 | N |
| ATOM | 958 | CA  | GLN | A | 133 | 0.998  | 14.739 | 37.663 | 1.00 | 58.15 | C |
| ATOM | 959 | C   | GLN | A | 133 | 0.172  | 15.450 | 38.751 | 1.00 | 58.99 | C |
| ATOM | 960 | O   | GLN | A | 133 | -0.915 | 15.950 | 38.470 | 1.00 | 58.73 | O |
| ATOM | 961 | CB  | GLN | A | 133 | 0.897  | 13.230 | 37.824 | 1.00 | 58.03 | C |
| ATOM | 962 | N   | ASP | A | 134 | 0.678  | 15.510 | 39.981 | 1.00 | 60.11 | N |
| ATOM | 963 | CA  | ASP | A | 134 | -0.081 | 16.145 | 41.063 | 1.00 | 61.49 | C |
| ATOM | 964 | C   | ASP | A | 134 | -0.362 | 17.629 | 40.783 | 1.00 | 61.55 | C |
| ATOM | 965 | O   | ASP | A | 134 | -1.427 | 18.149 | 41.104 | 1.00 | 61.55 | O |
| ATOM | 966 | CB  | ASP | A | 134 | 0.621  | 15.985 | 42.417 | 1.00 | 61.99 | C |
| ATOM | 967 | CG  | ASP | A | 134 | -0.253 | 16.454 | 43.587 | 1.00 | 64.74 | C |
| ATOM | 968 | OD1 | ASP | A | 134 | -1.310 | 17.082 | 43.346 | 1.00 | 67.52 | O |
| ATOM | 969 | OD2 | ASP | A | 134 | 0.022  | 16.237 | 44.791 | 1.00 | 69.05 | O |
| ATOM | 970 | N   | ILE | A | 135 | 0.594  | 18.312 | 40.179 | 1.00 | 61.80 | N |
| ATOM | 971 | CA  | ILE | A | 135 | 0.402  | 19.706 | 39.860 | 1.00 | 62.08 | C |
| ATOM | 972 | C   | ILE | A | 135 | -0.700 | 19.856 | 38.823 | 1.00 | 62.29 | C |
| ATOM | 973 | O   | ILE | A | 135 | -1.639 | 20.620 | 39.013 | 1.00 | 61.91 | O |
| ATOM | 974 | CB  | ILE | A | 135 | 1.711  | 20.301 | 39.366 | 1.00 | 62.21 | C |
| ATOM | 975 | CG1 | ILE | A | 135 | 2.705  | 20.391 | 40.528 | 1.00 | 62.47 | C |
| ATOM | 976 | CG2 | ILE | A | 135 | 1.478  | 21.670 | 38.783 | 1.00 | 62.19 | C |
| ATOM | 977 | CD1 | ILE | A | 135 | 4.157  | 20.437 | 40.100 | 1.00 | 62.96 | C |
| ATOM | 978 | N   | GLN | A | 136 | -0.593 | 19.112 | 37.733 | 1.00 | 62.99 | N |
| ATOM | 979 | CA  | GLN | A | 136 | -1.585 | 19.184 | 36.674 | 1.00 | 63.71 | C |
| ATOM | 980 | C   | GLN | A | 136 | -2.977 | 18.992 | 37.259 | 1.00 | 64.44 | C |
| ATOM | 981 | O   | GLN | A | 136 | -3.844 | 19.856 | 37.123 | 1.00 | 64.73 | O |
| ATOM | 982 | CB  | GLN | A | 136 | -1.305 | 18.136 | 35.619 | 1.00 | 63.77 | C |
| ATOM | 983 | N   | GLN | A | 137 | -3.170 | 17.871 | 37.948 | 1.00 | 65.12 | N |
| ATOM | 984 | CA  | GLN | A | 137 | -4.472 | 17.509 | 38.497 | 1.00 | 65.60 | C |
| ATOM | 985 | C   | GLN | A | 137 | -4.989 | 18.540 | 39.477 | 1.00 | 65.70 | C |
| ATOM | 986 | O   | GLN | A | 137 | -6.175 | 18.871 | 39.447 | 1.00 | 66.17 | O |
| ATOM | 987 | CB  | GLN | A | 137 | -4.421 | 16.117 | 39.161 | 1.00 | 65.72 | C |
| ATOM | 988 | N   | ARG | A | 138 | -4.115 | 19.056 | 40.336 | 1.00 | 65.61 | N |
| ATOM | 989 | CA  | ARG | A | 138 | -4.549 | 20.011 | 41.358 | 1.00 | 65.53 | C |
| ATOM | 990 | C   | ARG | A | 138 | -4.578 | 21.441 | 40.823 | 1.00 | 64.96 | C |
| ATOM | 991 | O   | ARG | A | 138 | -4.748 | 22.392 | 41.589 | 1.00 | 64.93 | O |
| ATOM | 992 | CB  | ARG | A | 138 | -3.670 | 19.912 | 42.613 | 1.00 | 65.65 | C |
| ATOM | 993 | CG  | ARG | A | 138 | -2.375 | 20.712 | 42.588 | 1.00 | 67.10 | C |
| ATOM | 994 | CD  | ARG | A | 138 | -1.482 | 20.352 | 43.745 | 1.00 | 68.96 | C |
| ATOM | 995 | NE  | ARG | A | 138 | -0.372 | 21.270 | 43.957 | 1.00 | 69.79 | N |
| ATOM | 996 | CZ  | ARG | A | 138 | 0.905  | 20.919 | 43.880 | 1.00 | 71.69 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 997  | NH1 | ARG | A | 138 | 1.238  | 19.674 | 43.569 | 1.00 | 72.88 | N |
| ATOM | 998  | NH2 | ARG | A | 138 | 1.862  | 21.811 | 44.106 | 1.00 | 72.52 | N |
| ATOM | 999  | N   | GLY | A | 139 | -4.426 | 21.593 | 39.508 | 1.00 | 64.31 | N |
| ATOM | 1000 | CA  | GLY | A | 139 | -4.370 | 22.912 | 38.897 | 1.00 | 63.53 | C |
| ATOM | 1001 | C   | GLY | A | 139 | -3.401 | 23.874 | 39.578 | 1.00 | 62.69 | C |
| ATOM | 1002 | O   | GLY | A | 139 | -3.631 | 25.080 | 39.570 | 1.00 | 62.92 | O |
| ATOM | 1003 | N   | GLY | A | 140 | -2.312 | 23.357 | 40.148 | 1.00 | 61.58 | N |
| ATOM | 1004 | CA  | GLY | A | 140 | -1.345 | 24.183 | 40.861 | 1.00 | 60.52 | C |
| ATOM | 1005 | C   | GLY | A | 140 | -0.539 | 25.103 | 39.958 | 1.00 | 59.56 | C |
| ATOM | 1006 | O   | GLY | A | 140 | -0.449 | 24.867 | 38.748 | 1.00 | 59.45 | O |
| ATOM | 1007 | N   | GLU | A | 141 | 0.041  | 26.159 | 40.530 | 1.00 | 58.05 | N |
| ATOM | 1008 | CA  | GLU | A | 141 | 0.859  | 27.090 | 39.748 | 1.00 | 56.92 | C |
| ATOM | 1009 | C   | GLU | A | 141 | 2.366  | 26.751 | 39.832 | 1.00 | 54.97 | C |
| ATOM | 1010 | O   | GLU | A | 141 | 3.189  | 27.326 | 39.113 | 1.00 | 54.51 | O |
| ATOM | 1011 | CB  | GLU | A | 141 | 0.602  | 28.547 | 40.177 | 1.00 | 57.45 | C |
| ATOM | 1012 | CG  | GLU | A | 141 | -0.707 | 29.171 | 39.680 | 1.00 | 59.67 | C |
| ATOM | 1013 | CD  | GLU | A | 141 | -0.851 | 29.193 | 38.154 | 1.00 | 63.48 | C |
| ATOM | 1014 | OE1 | GLU | A | 141 | 0.179  | 29.107 | 37.436 | 1.00 | 65.30 | O |
| ATOM | 1015 | OE2 | GLU | A | 141 | -2.007 | 29.298 | 37.664 | 1.00 | 66.13 | O |
| ATOM | 1016 | N   | GLU | A | 142 | 2.720  | 25.814 | 40.708 | 1.00 | 52.62 | N |
| ATOM | 1017 | CA  | GLU | A | 142 | 4.106  | 25.398 | 40.862 | 1.00 | 50.91 | C |
| ATOM | 1018 | C   | GLU | A | 142 | 4.679  | 24.958 | 39.516 | 1.00 | 48.93 | C |
| ATOM | 1019 | O   | GLU | A | 142 | 3.960  | 24.477 | 38.641 | 1.00 | 48.64 | O |
| ATOM | 1020 | CB  | GLU | A | 142 | 4.225  | 24.263 | 41.886 | 1.00 | 51.00 | C |
| ATOM | 1021 | CG  | GLU | A | 142 | 5.656  | 24.005 | 42.352 | 1.00 | 51.76 | C |
| ATOM | 1022 | CD  | GLU | A | 142 | 5.814  | 22.811 | 43.282 | 1.00 | 52.64 | C |
| ATOM | 1023 | OE1 | GLU | A | 142 | 4.871  | 22.009 | 43.447 | 1.00 | 55.52 | O |
| ATOM | 1024 | OE2 | GLU | A | 142 | 6.911  | 22.667 | 43.855 | 1.00 | 53.97 | O |
| ATOM | 1025 | N   | ARG | A | 143 | 5.979  | 25.139 | 39.356 | 1.00 | 46.58 | N |
| ATOM | 1026 | CA  | ARG | A | 143 | 6.652  | 24.751 | 38.133 | 1.00 | 45.12 | C |
| ATOM | 1027 | C   | ARG | A | 143 | 7.900  | 23.960 | 38.425 | 1.00 | 43.39 | C |
| ATOM | 1028 | O   | ARG | A | 143 | 8.616  | 24.242 | 39.387 | 1.00 | 43.58 | O |
| ATOM | 1029 | CB  | ARG | A | 143 | 7.069  | 25.983 | 37.360 | 1.00 | 45.52 | C |
| ATOM | 1030 | CG  | ARG | A | 143 | 5.943  | 26.747 | 36.729 | 1.00 | 45.38 | C |
| ATOM | 1031 | CD  | ARG | A | 143 | 6.488  | 27.899 | 35.969 | 1.00 | 46.06 | C |
| ATOM | 1032 | NE  | ARG | A | 143 | 5.473  | 28.649 | 35.252 | 1.00 | 45.33 | N |
| ATOM | 1033 | CZ  | ARG | A | 143 | 5.194  | 28.491 | 33.984 | 1.00 | 42.93 | C |
| ATOM | 1034 | NH1 | ARG | A | 143 | 5.836  | 27.573 | 33.253 | 1.00 | 41.86 | N |
| ATOM | 1035 | NH2 | ARG | A | 143 | 4.257  | 29.252 | 33.452 | 1.00 | 43.53 | N |
| ATOM | 1036 | N   | LEU | A | 144 | 8.182  | 22.991 | 37.578 | 1.00 | 41.08 | N |
| ATOM | 1037 | CA  | LEU | A | 144 | 9.337  | 22.163 | 37.784 | 1.00 | 39.63 | C |
| ATOM | 1038 | C   | LEU | A | 144 | 10.213 | 22.166 | 36.568 | 1.00 | 37.88 | C |
| ATOM | 1039 | O   | LEU | A | 144 | 9.734  | 22.249 | 35.444 | 1.00 | 36.26 | O |
| ATOM | 1040 | CB  | LEU | A | 144 | 8.889  | 20.727 | 38.018 | 1.00 | 40.26 | C |
| ATOM | 1041 | CG  | LEU | A | 144 | 7.974  | 20.529 | 39.223 | 1.00 | 41.73 | C |
| ATOM | 1042 | CD1 | LEU | A | 144 | 7.639  | 19.036 | 39.392 | 1.00 | 42.57 | C |
| ATOM | 1043 | CD2 | LEU | A | 144 | 8.585  | 21.102 | 40.503 | 1.00 | 41.42 | C |
| ATOM | 1044 | N   | TYR | A | 145 | 11.507 | 22.033 | 36.800 | 1.00 | 36.36 | N |
| ATOM | 1045 | CA  | TYR | A | 145 | 12.434 | 21.892 | 35.703 | 1.00 | 35.24 | C |
| ATOM | 1046 | C   | TYR | A | 145 | 13.485 | 20.862 | 36.107 | 1.00 | 34.89 | C |
| ATOM | 1047 | O   | TYR | A | 145 | 14.264 | 21.098 | 37.013 | 1.00 | 33.74 | O |
| ATOM | 1048 | CB  | TYR | A | 145 | 13.071 | 23.243 | 35.352 | 1.00 | 35.01 | C |
| ATOM | 1049 | CG  | TYR | A | 145 | 13.524 | 23.408 | 33.901 | 1.00 | 32.68 | C |
| ATOM | 1050 | CD1 | TYR | A | 145 | 13.817 | 22.324 | 33.099 | 1.00 | 30.20 | C |
| ATOM | 1051 | CD2 | TYR | A | 145 | 13.689 | 24.666 | 33.355 | 1.00 | 31.53 | C |
| ATOM | 1052 | CE1 | TYR | A | 145 | 14.237 | 22.493 | 31.762 | 1.00 | 29.87 | C |
| ATOM | 1053 | CE2 | TYR | A | 145 | 14.110 | 24.852 | 32.031 | 1.00 | 29.82 | C |
| ATOM | 1054 | CZ  | TYR | A | 145 | 14.373 | 23.765 | 31.228 | 1.00 | 30.06 | C |
| ATOM | 1055 | OH  | TYR | A | 145 | 14.789 | 23.953 | 29.897 | 1.00 | 28.17 | O |
| ATOM | 1056 | N   | LEU | A | 146 | 13.479 | 19.708 | 35.446 | 1.00 | 34.87 | N |
| ATOM | 1057 | CA  | LEU | A | 146 | 14.511 | 18.703 | 35.690 | 1.00 | 35.40 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1058 | C   | LEU | A | 146 | 15.753 | 18.977 | 34.864 | 1.00 | 35.24 | C |
| ATOM | 1059 | O   | LEU | A | 146 | 15.665 | 19.211 | 33.653 | 1.00 | 34.63 | O |
| ATOM | 1060 | CB  | LEU | A | 146 | 14.008 | 17.312 | 35.358 | 1.00 | 35.79 | C |
| ATOM | 1061 | CG  | LEU | A | 146 | 14.998 | 16.157 | 35.614 | 1.00 | 37.21 | C |
| ATOM | 1062 | CD1 | LEU | A | 146 | 14.221 | 14.918 | 35.969 | 1.00 | 36.28 | C |
| ATOM | 1063 | CD2 | LEU | A | 146 | 15.907 | 15.872 | 34.399 | 1.00 | 38.78 | C |
| ATOM | 1064 | N   | GLN | A | 147 | 16.907 | 18.883 | 35.515 | 1.00 | 34.82 | N |
| ATOM | 1065 | CA  | GLN | A | 147 | 18.179 | 19.206 | 34.884 | 1.00 | 35.00 | C |
| ATOM | 1066 | C   | GLN | A | 147 | 19.222 | 18.341 | 35.525 | 1.00 | 34.90 | C |
| ATOM | 1067 | O   | GLN | A | 147 | 19.626 | 18.568 | 36.664 | 1.00 | 35.65 | O |
| ATOM | 1068 | CB  | GLN | A | 147 | 18.526 | 20.679 | 35.078 | 1.00 | 35.09 | C |
| ATOM | 1069 | CG  | GLN | A | 147 | 17.392 | 21.636 | 34.720 | 1.00 | 35.83 | C |
| ATOM | 1070 | CD  | GLN | A | 147 | 17.848 | 23.085 | 34.706 | 1.00 | 36.90 | C |
| ATOM | 1071 | OE1 | GLN | A | 147 | 17.091 | 23.961 | 34.302 | 1.00 | 39.61 | O |
| ATOM | 1072 | NE2 | GLN | A | 147 | 19.088 | 23.336 | 35.126 | 1.00 | 35.05 | N |
| ATOM | 1073 | N   | GLN | A | 148 | 19.673 | 17.358 | 34.773 | 1.00 | 35.00 | N |
| ATOM | 1074 | CA  | GLN | A | 148 | 20.492 | 16.300 | 35.294 | 1.00 | 34.89 | C |
| ATOM | 1075 | C   | GLN | A | 148 | 21.376 | 15.709 | 34.255 | 1.00 | 35.35 | C |
| ATOM | 1076 | O   | GLN | A | 148 | 20.941 | 15.318 | 33.181 | 1.00 | 35.25 | O |
| ATOM | 1077 | CB  | GLN | A | 148 | 19.580 | 15.186 | 35.791 | 1.00 | 35.27 | C |
| ATOM | 1078 | CG  | GLN | A | 148 | 20.335 | 13.914 | 36.269 | 1.00 | 35.11 | C |
| ATOM | 1079 | CD  | GLN | A | 148 | 21.317 | 14.230 | 37.389 | 1.00 | 34.12 | C |
| ATOM | 1080 | OE1 | GLN | A | 148 | 20.998 | 15.033 | 38.277 | 1.00 | 33.18 | O |
| ATOM | 1081 | NE2 | GLN | A | 148 | 22.521 | 13.652 | 37.324 | 1.00 | 30.47 | N |
| ATOM | 1082 | N   | THR | A | 149 | 22.631 | 15.641 | 34.600 | 1.00 | 36.56 | N |
| ATOM | 1083 | CA  | THR | A | 149 | 23.648 | 15.088 | 33.754 | 1.00 | 38.26 | C |
| ATOM | 1084 | C   | THR | A | 149 | 23.394 | 13.609 | 33.615 | 1.00 | 38.31 | C |
| ATOM | 1085 | O   | THR | A | 149 | 23.068 | 12.956 | 34.597 | 1.00 | 38.70 | O |
| ATOM | 1086 | CB  | THR | A | 149 | 24.992 | 15.362 | 34.463 | 1.00 | 38.76 | C |
| ATOM | 1087 | OG1 | THR | A | 149 | 25.290 | 16.747 | 34.277 | 1.00 | 41.68 | O |
| ATOM | 1088 | CG2 | THR | A | 149 | 26.139 | 14.710 | 33.797 | 1.00 | 40.77 | C |
| ATOM | 1089 | N   | LEU | A | 150 | 23.516 | 13.087 | 32.399 | 1.00 | 38.77 | N |
| ATOM | 1090 | CA  | LEU | A | 150 | 23.373 | 11.664 | 32.149 | 1.00 | 39.27 | C |
| ATOM | 1091 | C   | LEU | A | 150 | 24.604 | 10.898 | 32.679 | 1.00 | 39.85 | C |
| ATOM | 1092 | O   | LEU | A | 150 | 25.733 | 11.207 | 32.321 | 1.00 | 39.99 | O |
| ATOM | 1093 | CB  | LEU | A | 150 | 23.220 | 11.402 | 30.660 | 1.00 | 39.15 | C |
| ATOM | 1094 | CG  | LEU | A | 150 | 21.943 | 11.860 | 29.962 | 1.00 | 40.72 | C |
| ATOM | 1095 | CD1 | LEU | A | 150 | 22.058 | 11.673 | 28.459 | 1.00 | 41.91 | C |
| ATOM | 1096 | CD2 | LEU | A | 150 | 20.764 | 11.106 | 30.458 | 1.00 | 41.30 | C |
| ATOM | 1097 | N   | ASN | A | 151 | 24.392 | 9.898  | 33.526 | 1.00 | 40.26 | N |
| ATOM | 1098 | CA  | ASN | A | 151 | 25.510 | 9.124  | 34.062 | 1.00 | 40.90 | C |
| ATOM | 1099 | C   | ASN | A | 151 | 25.291 | 7.607  | 34.041 | 1.00 | 41.95 | C |
| ATOM | 1100 | O   | ASN | A | 151 | 24.327 | 7.098  | 33.441 | 1.00 | 41.72 | O |
| ATOM | 1101 | CB  | ASN | A | 151 | 25.778 | 9.575  | 35.489 | 1.00 | 40.77 | C |
| ATOM | 1102 | CG  | ASN | A | 151 | 24.564 | 9.439  | 36.349 | 1.00 | 39.85 | C |
| ATOM | 1103 | OD1 | ASN | A | 151 | 24.002 | 8.340  | 36.483 | 1.00 | 37.92 | O |
| ATOM | 1104 | ND2 | ASN | A | 151 | 24.107 | 10.558 | 36.897 | 1.00 | 36.89 | N |
| ATOM | 1105 | N   | ASP | A | 152 | 26.176 | 6.894  | 34.735 | 1.00 | 42.89 | N |
| ATOM | 1106 | CA  | ASP | A | 152 | 26.175 | 5.431  | 34.756 | 1.00 | 43.75 | C |
| ATOM | 1107 | C   | ASP | A | 152 | 24.950 | 4.768  | 35.272 | 1.00 | 43.37 | C |
| ATOM | 1108 | O   | ASP | A | 152 | 24.787 | 3.581  | 35.052 | 1.00 | 43.66 | O |
| ATOM | 1109 | CB  | ASP | A | 152 | 27.256 | 4.895  | 35.695 | 1.00 | 44.77 | C |
| ATOM | 1110 | CG  | ASP | A | 152 | 28.539 | 5.555  | 35.500 | 1.00 | 48.22 | C |
| ATOM | 1111 | OD1 | ASP | A | 152 | 28.835 | 5.881  | 34.325 | 1.00 | 57.47 | O |
| ATOM | 1112 | OD2 | ASP | A | 152 | 29.291 | 5.826  | 36.437 | 1.00 | 51.28 | O |
| ATOM | 1113 | N   | THR | A | 153 | 24.119 | 5.466  | 36.025 | 1.00 | 43.41 | N |
| ATOM | 1114 | CA  | THR | A | 153 | 22.983 | 4.783  | 36.631 | 1.00 | 43.38 | C |
| ATOM | 1115 | C   | THR | A | 153 | 21.820 | 4.605  | 35.676 | 1.00 | 42.99 | C |
| ATOM | 1116 | O   | THR | A | 153 | 20.866 | 3.945  | 36.012 | 1.00 | 43.44 | O |
| ATOM | 1117 | CB  | THR | A | 153 | 22.489 | 5.507  | 37.875 | 1.00 | 43.44 | C |
| ATOM | 1118 | OG1 | THR | A | 153 | 21.749 | 6.678  | 37.499 | 1.00 | 46.09 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1119 | CG2 | THR | A | 153 | 23.651 | 6.008  | 38.725 | 1.00 | 42.99 | C |
| ATOM | 1120 | N   | VAL | A | 154 | 21.874 | 5.185  | 34.491 | 1.00 | 42.88 | N |
| ATOM | 1121 | CA  | VAL | A | 154 | 20.757 | 5.015  | 33.572 | 1.00 | 42.71 | C |
| ATOM | 1122 | C   | VAL | A | 154 | 20.700 | 3.563  | 33.177 | 1.00 | 42.42 | C |
| ATOM | 1123 | O   | VAL | A | 154 | 21.729 | 2.892  | 33.193 | 1.00 | 42.39 | O |
| ATOM | 1124 | CB  | VAL | A | 154 | 20.889 | 5.875  | 32.300 | 1.00 | 42.67 | C |
| ATOM | 1125 | CG1 | VAL | A | 154 | 20.857 | 7.347  | 32.660 | 1.00 | 43.04 | C |
| ATOM | 1126 | CG2 | VAL | A | 154 | 22.159 | 5.516  | 31.538 | 1.00 | 42.56 | C |
| ATOM | 1127 | N   | GLY | A | 155 | 19.502 | 3.097  | 32.814 | 1.00 | 42.11 | N |
| ATOM | 1128 | CA  | GLY | A | 155 | 19.261 | 1.725  | 32.411 | 1.00 | 41.52 | C |
| ATOM | 1129 | C   | GLY | A | 155 | 19.642 | 1.317  | 30.992 | 1.00 | 41.85 | C |
| ATOM | 1130 | O   | GLY | A | 155 | 19.977 | 2.140  | 30.123 | 1.00 | 41.87 | O |
| ATOM | 1131 | N   | ARG | A | 156 | 19.512 | 0.012  | 30.750 | 1.00 | 41.36 | N |
| ATOM | 1132 | CA  | ARG | A | 156 | 19.961 | -0.623 | 29.511 | 1.00 | 40.88 | C |
| ATOM | 1133 | C   | ARG | A | 156 | 19.397 | -0.005 | 28.247 | 1.00 | 40.03 | C |
| ATOM | 1134 | O   | ARG | A | 156 | 20.135 | 0.304  | 27.339 | 1.00 | 40.36 | O |
| ATOM | 1135 | CB  | ARG | A | 156 | 19.670 | -2.148 | 29.555 | 1.00 | 40.77 | C |
| ATOM | 1136 | N   | LYS | A | 157 | 18.090 | 0.146  | 28.181 | 1.00 | 39.16 | N |
| ATOM | 1137 | CA  | LYS | A | 157 | 17.503 | 0.697  | 26.990 | 1.00 | 38.81 | C |
| ATOM | 1138 | C   | LYS | A | 157 | 18.078 | 2.114  | 26.738 | 1.00 | 38.38 | C |
| ATOM | 1139 | O   | LYS | A | 157 | 18.363 | 2.464  | 25.594 | 1.00 | 37.97 | O |
| ATOM | 1140 | CB  | LYS | A | 157 | 15.968 | 0.714  | 27.090 | 1.00 | 39.20 | C |
| ATOM | 1141 | CG  | LYS | A | 157 | 15.266 | -0.575 | 26.642 | 1.00 | 36.80 | C |
| ATOM | 1142 | N   | ILE | A | 158 | 18.268 | 2.909  | 27.791 | 1.00 | 37.56 | N |
| ATOM | 1143 | CA  | ILE | A | 158 | 18.759 | 4.287  | 27.606 | 1.00 | 37.28 | C |
| ATOM | 1144 | C   | ILE | A | 158 | 20.180 | 4.281  | 27.126 | 1.00 | 37.22 | C |
| ATOM | 1145 | O   | ILE | A | 158 | 20.582 | 5.120  | 26.302 | 1.00 | 37.08 | O |
| ATOM | 1146 | CB  | ILE | A | 158 | 18.692 | 5.101  | 28.882 | 1.00 | 36.72 | C |
| ATOM | 1147 | CG1 | ILE | A | 158 | 17.257 | 5.220  | 29.356 | 1.00 | 37.17 | C |
| ATOM | 1148 | CG2 | ILE | A | 158 | 19.254 | 6.465  | 28.646 | 1.00 | 36.48 | C |
| ATOM | 1149 | CD1 | ILE | A | 158 | 16.359 | 5.900  | 28.409 | 1.00 | 38.28 | C |
| ATOM | 1150 | N   | VAL | A | 159 | 20.934 | 3.335  | 27.655 | 1.00 | 36.85 | N |
| ATOM | 1151 | CA  | VAL | A | 159 | 22.319 | 3.177  | 27.284 | 1.00 | 37.05 | C |
| ATOM | 1152 | C   | VAL | A | 159 | 22.349 | 2.864  | 25.785 | 1.00 | 36.45 | C |
| ATOM | 1153 | O   | VAL | A | 159 | 23.165 | 3.410  | 25.057 | 1.00 | 35.81 | O |
| ATOM | 1154 | CB  | VAL | A | 159 | 22.988 | 2.042  | 28.096 | 1.00 | 37.36 | C |
| ATOM | 1155 | CG1 | VAL | A | 159 | 24.248 | 1.567  | 27.427 | 1.00 | 38.43 | C |
| ATOM | 1156 | CG2 | VAL | A | 159 | 23.302 | 2.499  | 29.494 | 1.00 | 37.81 | C |
| ATOM | 1157 | N   | MET | A | 160 | 21.453 | 1.990  | 25.339 | 1.00 | 35.84 | N |
| ATOM | 1158 | CA  | MET | A | 160 | 21.369 | 1.637  | 23.910 | 1.00 | 36.30 | C |
| ATOM | 1159 | C   | MET | A | 160 | 21.064 | 2.883  | 23.074 | 1.00 | 34.46 | C |
| ATOM | 1160 | O   | MET | A | 160 | 21.715 | 3.142  | 22.083 | 1.00 | 33.88 | O |
| ATOM | 1161 | CB  | MET | A | 160 | 20.294 | 0.576  | 23.656 | 1.00 | 36.83 | C |
| ATOM | 1162 | CG  | MET | A | 160 | 20.654 | -0.763 | 24.225 | 1.00 | 39.89 | C |
| ATOM | 1163 | SD  | MET | A | 160 | 21.916 | -1.579 | 23.249 | 1.00 | 46.87 | S |
| ATOM | 1164 | CE  | MET | A | 160 | 21.005 | -1.940 | 21.669 | 1.00 | 47.08 | C |
| ATOM | 1165 | N   | ASP | A | 161 | 20.078 | 3.648  | 23.505 | 1.00 | 33.13 | N |
| ATOM | 1166 | CA  | ASP | A | 161 | 19.732 | 4.901  | 22.857 | 1.00 | 32.80 | C |
| ATOM | 1167 | C   | ASP | A | 161 | 20.931 | 5.877  | 22.747 | 1.00 | 31.75 | C |
| ATOM | 1168 | O   | ASP | A | 161 | 21.209 | 6.425  | 21.691 | 1.00 | 31.06 | O |
| ATOM | 1169 | CB  | ASP | A | 161 | 18.598 | 5.553  | 23.631 | 1.00 | 32.93 | C |
| ATOM | 1170 | CG  | ASP | A | 161 | 17.278 | 4.822  | 23.473 | 1.00 | 33.90 | C |
| ATOM | 1171 | OD1 | ASP | A | 161 | 17.148 | 3.961  | 22.568 | 1.00 | 28.71 | O |
| ATOM | 1172 | OD2 | ASP | A | 161 | 16.301 | 5.064  | 24.226 | 1.00 | 38.17 | O |
| ATOM | 1173 | N   | PHE | A | 162 | 21.646 | 6.052  | 23.849 | 1.00 | 31.05 | N |
| ATOM | 1174 | CA  | PHE | A | 162 | 22.763 | 6.968  | 23.930 | 1.00 | 30.52 | C |
| ATOM | 1175 | C   | PHE | A | 162 | 23.835 | 6.553  | 22.979 | 1.00 | 28.89 | C |
| ATOM | 1176 | O   | PHE | A | 162 | 24.477 | 7.369  | 22.371 | 1.00 | 29.43 | O |
| ATOM | 1177 | CB  | PHE | A | 162 | 23.311 | 6.948  | 25.375 | 1.00 | 30.80 | C |
| ATOM | 1178 | CG  | PHE | A | 162 | 24.493 | 7.839  | 25.617 | 1.00 | 31.81 | C |
| ATOM | 1179 | CD1 | PHE | A | 162 | 24.325 | 9.179  | 25.904 | 1.00 | 35.81 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1180 | CD2 | PHE | A | 162 | 25.770 | 7.322  | 25.653 | 1.00 | 35.00 | C |
| ATOM | 1181 | CE1 | PHE | A | 162 | 25.430 | 10.000 | 26.197 | 1.00 | 35.94 | C |
| ATOM | 1182 | CE2 | PHE | A | 162 | 26.887 | 8.143  | 25.941 | 1.00 | 35.90 | C |
| ATOM | 1183 | CZ  | PHE | A | 162 | 26.711 | 9.467  | 26.202 | 1.00 | 35.61 | C |
| ATOM | 1184 | N   | LEU | A | 163 | 24.067 | 5.271  | 22.914 | 1.00 | 28.19 | N |
| ATOM | 1185 | CA  | LEU | A | 163 | 25.103 | 4.728  | 22.065 | 1.00 | 28.08 | C |
| ATOM | 1186 | C   | LEU | A | 163 | 24.735 | 4.923  | 20.590 | 1.00 | 27.13 | C |
| ATOM | 1187 | O   | LEU | A | 163 | 25.603 | 4.973  | 19.751 | 1.00 | 26.83 | O |
| ATOM | 1188 | CB  | LEU | A | 163 | 25.306 | 3.244  | 22.368 | 1.00 | 27.86 | C |
| ATOM | 1189 | CG  | LEU | A | 163 | 26.137 | 2.987  | 23.604 | 1.00 | 28.73 | C |
| ATOM | 1190 | CD1 | LEU | A | 163 | 26.180 | 1.512  | 23.849 | 1.00 | 29.77 | C |
| ATOM | 1191 | CD2 | LEU | A | 163 | 27.559 | 3.522  | 23.464 | 1.00 | 29.70 | C |
| ATOM | 1192 | N   | GLY | A | 164 | 23.448 | 4.998  | 20.303 | 1.00 | 26.50 | N |
| ATOM | 1193 | CA  | GLY | A | 164 | 22.956 | 5.244  | 18.959 | 1.00 | 27.37 | C |
| ATOM | 1194 | C   | GLY | A | 164 | 22.949 | 6.712  | 18.493 | 1.00 | 27.88 | C |
| ATOM | 1195 | O   | GLY | A | 164 | 22.483 | 6.988  | 17.365 | 1.00 | 28.42 | O |
| ATOM | 1196 | N   | PHE | A | 165 | 23.420 | 7.635  | 19.344 | 1.00 | 26.36 | N |
| ATOM | 1197 | CA  | PHE | A | 165 | 23.530 | 9.011  | 18.958 | 1.00 | 26.57 | C |
| ATOM | 1198 | C   | PHE | A | 165 | 24.540 | 9.052  | 17.820 | 1.00 | 26.12 | C |
| ATOM | 1199 | O   | PHE | A | 165 | 25.381 | 8.202  | 17.756 | 1.00 | 24.23 | O |
| ATOM | 1200 | CB  | PHE | A | 165 | 24.024 | 9.867  | 20.153 | 1.00 | 26.86 | C |
| ATOM | 1201 | CG  | PHE | A | 165 | 22.979 | 10.070 | 21.252 | 1.00 | 27.80 | C |
| ATOM | 1202 | CD1 | PHE | A | 165 | 21.701 | 9.533  | 21.144 | 1.00 | 27.80 | C |
| ATOM | 1203 | CD2 | PHE | A | 165 | 23.274 | 10.820 | 22.367 | 1.00 | 28.58 | C |
| ATOM | 1204 | CE1 | PHE | A | 165 | 20.765 | 9.744  | 22.117 | 1.00 | 26.89 | C |
| ATOM | 1205 | CE2 | PHE | A | 165 | 22.329 | 11.042 | 23.364 | 1.00 | 28.45 | C |
| ATOM | 1206 | CZ  | PHE | A | 165 | 21.086 | 10.504 | 23.243 | 1.00 | 28.78 | C |
| ATOM | 1207 | N   | ASN | A | 166 | 24.496 | 10.077 | 16.963 | 1.00 | 26.15 | N |
| ATOM | 1208 | CA  | ASN | A | 166 | 25.441 | 10.165 | 15.837 | 1.00 | 25.91 | C |
| ATOM | 1209 | C   | ASN | A | 166 | 26.861 | 10.675 | 16.226 | 1.00 | 26.12 | C |
| ATOM | 1210 | O   | ASN | A | 166 | 27.288 | 11.793 | 15.894 | 1.00 | 25.48 | O |
| ATOM | 1211 | CB  | ASN | A | 166 | 24.834 | 11.004 | 14.705 | 1.00 | 25.51 | C |
| ATOM | 1212 | CG  | ASN | A | 166 | 25.634 | 10.916 | 13.431 | 1.00 | 24.43 | C |
| ATOM | 1213 | OD1 | ASN | A | 166 | 26.751 | 10.323 | 13.429 | 1.00 | 23.40 | O |
| ATOM | 1214 | ND2 | ASN | A | 166 | 25.078 | 11.479 | 12.318 | 1.00 | 17.22 | N |
| ATOM | 1215 | N   | TRP | A | 167 | 27.566 | 9.817  | 16.940 | 1.00 | 26.11 | N |
| ATOM | 1216 | CA  | TRP | A | 167 | 28.907 | 10.080 | 17.401 | 1.00 | 26.58 | C |
| ATOM | 1217 | C   | TRP | A | 167 | 29.817 | 10.336 | 16.206 | 1.00 | 27.07 | C |
| ATOM | 1218 | O   | TRP | A | 167 | 30.737 | 11.139 | 16.252 | 1.00 | 26.92 | O |
| ATOM | 1219 | CB  | TRP | A | 167 | 29.389 | 8.860  | 18.249 | 1.00 | 26.02 | C |
| ATOM | 1220 | CG  | TRP | A | 167 | 28.537 | 8.750  | 19.498 | 1.00 | 27.18 | C |
| ATOM | 1221 | CD1 | TRP | A | 167 | 27.620 | 7.784  | 19.809 | 1.00 | 28.08 | C |
| ATOM | 1222 | CD2 | TRP | A | 167 | 28.452 | 9.719  | 20.550 | 1.00 | 27.33 | C |
| ATOM | 1223 | NE1 | TRP | A | 167 | 27.013 | 8.071  | 21.013 | 1.00 | 27.87 | N |
| ATOM | 1224 | CE2 | TRP | A | 167 | 27.503 | 9.254  | 21.481 | 1.00 | 26.46 | C |
| ATOM | 1225 | CE3 | TRP | A | 167 | 29.103 | 10.929 | 20.804 | 1.00 | 26.22 | C |
| ATOM | 1226 | CZ2 | TRP | A | 167 | 27.180 | 9.951  | 22.622 | 1.00 | 28.27 | C |
| ATOM | 1227 | CZ3 | TRP | A | 167 | 28.784 | 11.615 | 21.920 | 1.00 | 27.56 | C |
| ATOM | 1228 | CH2 | TRP | A | 167 | 27.821 | 11.128 | 22.833 | 1.00 | 28.04 | C |
| ATOM | 1229 | N   | ASN | A | 168 | 29.585 | 9.632  | 15.114 | 1.00 | 27.98 | N |
| ATOM | 1230 | CA  | ASN | A | 168 | 30.430 | 9.833  | 13.959 | 1.00 | 28.32 | C |
| ATOM | 1231 | C   | ASN | A | 168 | 30.470 | 11.319 | 13.573 | 1.00 | 29.00 | C |
| ATOM | 1232 | O   | ASN | A | 168 | 31.547 | 11.894 | 13.390 | 1.00 | 30.41 | O |
| ATOM | 1233 | CB  | ASN | A | 168 | 29.909 | 9.018  | 12.812 | 1.00 | 28.58 | C |
| ATOM | 1234 | CG  | ASN | A | 168 | 30.758 | 9.145  | 11.570 | 1.00 | 29.28 | C |
| ATOM | 1235 | OD1 | ASN | A | 168 | 31.899 | 8.739  | 11.579 | 1.00 | 30.27 | O |
| ATOM | 1236 | ND2 | ASN | A | 168 | 30.186 | 9.677  | 10.487 | 1.00 | 28.46 | N |
| ATOM | 1237 | N   | TRP | A | 169 | 29.301 | 11.942 | 13.462 | 1.00 | 27.93 | N |
| ATOM | 1238 | CA  | TRP | A | 169 | 29.228 | 13.343 | 13.074 | 1.00 | 27.25 | C |
| ATOM | 1239 | C   | TRP | A | 169 | 29.726 | 14.266 | 14.179 | 1.00 | 27.20 | C |
| ATOM | 1240 | O   | TRP | A | 169 | 30.444 | 15.224 | 13.925 | 1.00 | 26.30 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1241 | CB  | TRP | A | 169 | 27.777 | 13.734 | 12.691 | 1.00 | 26.63 | C |
| ATOM | 1242 | CG  | TRP | A | 169 | 27.615 | 15.168 | 12.355 | 1.00 | 25.15 | C |
| ATOM | 1243 | CD1 | TRP | A | 169 | 27.804 | 15.745 | 11.130 | 1.00 | 24.89 | C |
| ATOM | 1244 | CD2 | TRP | A | 169 | 27.261 | 16.229 | 13.237 | 1.00 | 23.66 | C |
| ATOM | 1245 | NE1 | TRP | A | 169 | 27.591 | 17.095 | 11.195 | 1.00 | 22.98 | N |
| ATOM | 1246 | CE2 | TRP | A | 169 | 27.257 | 17.427 | 12.476 | 1.00 | 25.81 | C |
| ATOM | 1247 | CE3 | TRP | A | 169 | 26.927 | 16.292 | 14.576 | 1.00 | 24.44 | C |
| ATOM | 1248 | CZ2 | TRP | A | 169 | 26.933 | 18.680 | 13.018 | 1.00 | 26.96 | C |
| ATOM | 1249 | CZ3 | TRP | A | 169 | 26.624 | 17.525 | 15.127 | 1.00 | 28.68 | C |
| ATOM | 1250 | CH2 | TRP | A | 169 | 26.611 | 18.710 | 14.336 | 1.00 | 28.73 | C |
| ATOM | 1251 | N   | ILE | A | 170 | 29.323 | 14.026 | 15.409 | 1.00 | 27.29 | N |
| ATOM | 1252 | CA  | ILE | A | 170 | 29.725 | 14.985 | 16.406 | 1.00 | 28.36 | C |
| ATOM | 1253 | C   | ILE | A | 170 | 31.252 | 14.874 | 16.686 | 1.00 | 29.15 | C |
| ATOM | 1254 | O   | ILE | A | 170 | 31.920 | 15.875 | 16.866 | 1.00 | 29.81 | O |
| ATOM | 1255 | CB  | ILE | A | 170 | 28.814 | 14.947 | 17.672 | 1.00 | 28.10 | C |
| ATOM | 1256 | CG1 | ILE | A | 170 | 28.882 | 16.277 | 18.386 | 1.00 | 26.98 | C |
| ATOM | 1257 | CG2 | ILE | A | 170 | 29.198 | 13.838 | 18.593 | 1.00 | 27.15 | C |
| ATOM | 1258 | CD1 | ILE | A | 170 | 27.855 | 16.400 | 19.530 | 1.00 | 28.88 | C |
| ATOM | 1259 | N   | ASN | A | 171 | 31.809 | 13.679 | 16.653 | 1.00 | 29.35 | N |
| ATOM | 1260 | CA  | ASN | A | 171 | 33.261 | 13.535 | 16.843 | 1.00 | 30.18 | C |
| ATOM | 1261 | C   | ASN | A | 171 | 34.060 | 14.259 | 15.752 | 1.00 | 30.67 | C |
| ATOM | 1262 | O   | ASN | A | 171 | 35.117 | 14.823 | 16.036 | 1.00 | 31.32 | O |
| ATOM | 1263 | CB  | ASN | A | 171 | 33.705 | 12.058 | 16.861 | 1.00 | 29.80 | C |
| ATOM | 1264 | CG  | ASN | A | 171 | 33.210 | 11.274 | 18.094 | 1.00 | 30.17 | C |
| ATOM | 1265 | OD1 | ASN | A | 171 | 32.682 | 11.821 | 19.051 | 1.00 | 30.65 | O |
| ATOM | 1266 | ND2 | ASN | A | 171 | 33.372 | 9.968  | 18.036 | 1.00 | 31.44 | N |
| ATOM | 1267 | N   | LYS | A | 172 | 33.591 | 14.231 | 14.509 | 1.00 | 30.94 | N |
| ATOM | 1268 | CA  | LYS | A | 172 | 34.297 | 14.960 | 13.461 | 1.00 | 32.29 | C |
| ATOM | 1269 | C   | LYS | A | 172 | 34.211 | 16.473 | 13.755 | 1.00 | 31.79 | C |
| ATOM | 1270 | O   | LYS | A | 172 | 35.128 | 17.234 | 13.482 | 1.00 | 32.06 | O |
| ATOM | 1271 | CB  | LYS | A | 172 | 33.754 | 14.646 | 12.055 | 1.00 | 32.47 | C |
| ATOM | 1272 | CG  | LYS | A | 172 | 34.168 | 13.298 | 11.539 | 1.00 | 36.36 | C |
| ATOM | 1273 | CD  | LYS | A | 172 | 33.697 | 13.012 | 10.072 | 1.00 | 41.05 | C |
| ATOM | 1274 | CE  | LYS | A | 172 | 34.338 | 11.721 | 9.543  | 1.00 | 44.14 | C |
| ATOM | 1275 | NZ  | LYS | A | 172 | 34.321 | 11.571 | 8.024  | 1.00 | 49.11 | N |
| ATOM | 1276 | N   | GLN | A | 173 | 33.099 | 16.900 | 14.316 | 1.00 | 31.59 | N |
| ATOM | 1277 | CA  | GLN | A | 173 | 32.931 | 18.299 | 14.616 | 1.00 | 31.80 | C |
| ATOM | 1278 | C   | GLN | A | 173 | 33.965 | 18.680 | 15.681 | 1.00 | 32.04 | C |
| ATOM | 1279 | O   | GLN | A | 173 | 34.670 | 19.687 | 15.534 | 1.00 | 32.67 | O |
| ATOM | 1280 | CB  | GLN | A | 173 | 31.522 | 18.581 | 15.117 | 1.00 | 31.45 | C |
| ATOM | 1281 | CG  | GLN | A | 173 | 30.477 | 18.685 | 14.067 | 1.00 | 31.68 | C |
| ATOM | 1282 | CD  | GLN | A | 173 | 30.782 | 19.751 | 13.050 | 1.00 | 32.76 | C |
| ATOM | 1283 | OE1 | GLN | A | 173 | 31.198 | 20.852 | 13.405 | 1.00 | 36.55 | O |
| ATOM | 1284 | NE2 | GLN | A | 173 | 30.583 | 19.440 | 11.790 | 1.00 | 32.28 | N |
| ATOM | 1285 | N   | GLN | A | 174 | 34.044 | 17.871 | 16.735 | 1.00 | 31.40 | N |
| ATOM | 1286 | CA  | GLN | A | 174 | 34.999 | 18.074 | 17.811 | 1.00 | 31.28 | C |
| ATOM | 1287 | C   | GLN | A | 174 | 36.437 | 18.098 | 17.244 | 1.00 | 30.94 | C |
| ATOM | 1288 | O   | GLN | A | 174 | 37.253 | 18.939 | 17.602 | 1.00 | 30.50 | O |
| ATOM | 1289 | CB  | GLN | A | 174 | 34.808 | 16.971 | 18.861 | 1.00 | 31.20 | C |
| ATOM | 1290 | CG  | GLN | A | 174 | 35.859 | 16.917 | 19.935 | 1.00 | 31.64 | C |
| ATOM | 1291 | CD  | GLN | A | 174 | 35.704 | 15.717 | 20.836 | 1.00 | 31.52 | C |
| ATOM | 1292 | OE1 | GLN | A | 174 | 35.313 | 14.661 | 20.382 | 1.00 | 35.10 | O |
| ATOM | 1293 | NE2 | GLN | A | 174 | 36.007 | 15.880 | 22.121 | 1.00 | 32.92 | N |
| ATOM | 1294 | N   | GLY | A | 175 | 36.732 | 17.202 | 16.317 | 1.00 | 30.54 | N |
| ATOM | 1295 | CA  | GLY | A | 175 | 38.048 | 17.169 | 15.721 | 1.00 | 30.38 | C |
| ATOM | 1296 | C   | GLY | A | 175 | 38.288 | 18.339 | 14.783 | 1.00 | 31.21 | C |
| ATOM | 1297 | O   | GLY | A | 175 | 39.339 | 18.974 | 14.812 | 1.00 | 31.31 | O |
| ATOM | 1298 | N   | LYS | A | 176 | 37.317 | 18.661 | 13.946 | 1.00 | 31.67 | N |
| ATOM | 1299 | CA  | LYS | A | 176 | 37.524 | 19.767 | 13.029 | 1.00 | 32.84 | C |
| ATOM | 1300 | C   | LYS | A | 176 | 37.758 | 21.127 | 13.749 | 1.00 | 32.90 | C |
| ATOM | 1301 | O   | LYS | A | 176 | 38.563 | 21.906 | 13.291 | 1.00 | 32.85 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1302 | CB  | LYS | A | 176 | 36.351 | 19.915 | 12.074 | 1.00 | 33.80 | C |
| ATOM | 1303 | CG  | LYS | A | 176 | 36.187 | 18.832 | 11.037 | 1.00 | 35.93 | C |
| ATOM | 1304 | CD  | LYS | A | 176 | 34.982 | 19.185 | 10.168 | 1.00 | 39.44 | C |
| ATOM | 1305 | CE  | LYS | A | 176 | 34.055 | 18.032 | 9.961  | 1.00 | 40.94 | C |
| ATOM | 1306 | NZ  | LYS | A | 176 | 32.686 | 18.495 | 9.578  | 1.00 | 45.01 | N |
| ATOM | 1307 | N   | ARG | A | 177 | 37.074 | 21.398 | 14.859 | 1.00 | 32.98 | N |
| ATOM | 1308 | CA  | ARG | A | 177 | 37.242 | 22.677 | 15.571 | 1.00 | 33.61 | C |
| ATOM | 1309 | C   | ARG | A | 177 | 38.313 | 22.713 | 16.678 | 1.00 | 33.16 | C |
| ATOM | 1310 | O   | ARG | A | 177 | 38.453 | 23.717 | 17.370 | 1.00 | 33.01 | O |
| ATOM | 1311 | CB  | ARG | A | 177 | 35.920 | 23.101 | 16.220 | 1.00 | 33.86 | C |
| ATOM | 1312 | CG  | ARG | A | 177 | 34.716 | 22.947 | 15.353 | 1.00 | 35.87 | C |
| ATOM | 1313 | CD  | ARG | A | 177 | 34.728 | 23.721 | 14.062 | 1.00 | 37.56 | C |
| ATOM | 1314 | NE  | ARG | A | 177 | 33.704 | 23.135 | 13.222 | 1.00 | 42.96 | N |
| ATOM | 1315 | CZ  | ARG | A | 177 | 33.803 | 22.893 | 11.928 | 1.00 | 45.93 | C |
| ATOM | 1316 | NH1 | ARG | A | 177 | 34.897 | 23.218 | 11.247 | 1.00 | 46.65 | N |
| ATOM | 1317 | NH2 | ARG | A | 177 | 32.770 | 22.349 | 11.304 | 1.00 | 47.47 | N |
| ATOM | 1318 | N   | GLY | A | 178 | 39.038 | 21.624 | 16.887 | 1.00 | 32.79 | N |
| ATOM | 1319 | CA  | GLY | A | 178 | 40.068 | 21.629 | 17.907 | 1.00 | 31.78 | C |
| ATOM | 1320 | C   | GLY | A | 178 | 39.511 | 21.614 | 19.313 | 1.00 | 31.64 | C |
| ATOM | 1321 | O   | GLY | A | 178 | 40.251 | 21.782 | 20.292 | 1.00 | 33.25 | O |
| ATOM | 1322 | N   | TRP | A | 179 | 38.223 | 21.380 | 19.468 | 1.00 | 30.56 | N |
| ATOM | 1323 | CA  | TRP | A | 179 | 37.690 | 21.361 | 20.821 | 1.00 | 30.44 | C |
| ATOM | 1324 | C   | TRP | A | 179 | 38.328 | 20.385 | 21.789 | 1.00 | 30.36 | C |
| ATOM | 1325 | O   | TRP | A | 179 | 39.008 | 19.446 | 21.416 | 1.00 | 29.60 | O |
| ATOM | 1326 | CB  | TRP | A | 179 | 36.200 | 21.115 | 20.806 | 1.00 | 30.43 | C |
| ATOM | 1327 | CG  | TRP | A | 179 | 35.426 | 22.183 | 20.136 | 1.00 | 29.86 | C |
| ATOM | 1328 | CD1 | TRP | A | 179 | 35.882 | 23.409 | 19.721 | 1.00 | 27.42 | C |
| ATOM | 1329 | CD2 | TRP | A | 179 | 34.054 | 22.115 | 19.769 | 1.00 | 29.51 | C |
| ATOM | 1330 | NE1 | TRP | A | 179 | 34.870 | 24.102 | 19.104 | 1.00 | 30.05 | N |
| ATOM | 1331 | CE2 | TRP | A | 179 | 33.728 | 23.338 | 19.130 | 1.00 | 30.70 | C |
| ATOM | 1332 | CE3 | TRP | A | 179 | 33.067 | 21.145 | 19.902 | 1.00 | 27.24 | C |
| ATOM | 1333 | CZ2 | TRP | A | 179 | 32.470 | 23.602 | 18.626 | 1.00 | 27.82 | C |
| ATOM | 1334 | CZ3 | TRP | A | 179 | 31.829 | 21.397 | 19.389 | 1.00 | 28.43 | C |
| ATOM | 1335 | CH2 | TRP | A | 179 | 31.532 | 22.630 | 18.759 | 1.00 | 29.15 | C |
| ATOM | 1336 | N   | GLY | A | 180 | 38.087 | 20.634 | 23.065 | 1.00 | 30.98 | N |
| ATOM | 1337 | CA  | GLY | A | 180 | 38.515 | 19.723 | 24.104 | 1.00 | 30.78 | C |
| ATOM | 1338 | C   | GLY | A | 180 | 37.468 | 18.637 | 24.246 | 1.00 | 31.74 | C |
| ATOM | 1339 | O   | GLY | A | 180 | 36.621 | 18.448 | 23.343 | 1.00 | 31.97 | O |
| ATOM | 1340 | N   | GLN | A | 181 | 37.498 | 17.941 | 25.378 | 1.00 | 32.16 | N |
| ATOM | 1341 | CA  | GLN | A | 181 | 36.628 | 16.798 | 25.608 | 1.00 | 33.12 | C |
| ATOM | 1342 | C   | GLN | A | 181 | 35.161 | 17.108 | 25.885 | 1.00 | 32.52 | C |
| ATOM | 1343 | O   | GLN | A | 181 | 34.813 | 18.181 | 26.348 | 1.00 | 32.55 | O |
| ATOM | 1344 | CB  | GLN | A | 181 | 37.161 | 15.962 | 26.773 | 1.00 | 33.24 | C |
| ATOM | 1345 | CG  | GLN | A | 181 | 36.780 | 16.496 | 28.155 | 1.00 | 37.52 | C |
| ATOM | 1346 | CD  | GLN | A | 181 | 37.066 | 15.488 | 29.282 | 1.00 | 42.63 | C |
| ATOM | 1347 | OE1 | GLN | A | 181 | 38.200 | 15.034 | 29.442 | 1.00 | 46.67 | O |
| ATOM | 1348 | NE2 | GLN | A | 181 | 36.037 | 15.131 | 30.043 | 1.00 | 45.13 | N |
| ATOM | 1349 | N   | LEU | A | 182 | 34.310 | 16.134 | 25.588 | 1.00 | 32.12 | N |
| ATOM | 1350 | CA  | LEU | A | 182 | 32.907 | 16.155 | 26.001 | 1.00 | 31.88 | C |
| ATOM | 1351 | C   | LEU | A | 182 | 32.928 | 16.114 | 27.528 | 1.00 | 30.66 | C |
| ATOM | 1352 | O   | LEU | A | 182 | 33.481 | 15.190 | 28.087 | 1.00 | 30.31 | O |
| ATOM | 1353 | CB  | LEU | A | 182 | 32.228 | 14.880 | 25.512 | 1.00 | 31.80 | C |
| ATOM | 1354 | CG  | LEU | A | 182 | 30.715 | 14.723 | 25.454 | 1.00 | 33.59 | C |
| ATOM | 1355 | CD1 | LEU | A | 182 | 30.319 | 13.250 | 25.572 | 1.00 | 32.15 | C |
| ATOM | 1356 | CD2 | LEU | A | 182 | 30.059 | 15.454 | 26.520 | 1.00 | 36.60 | C |
| ATOM | 1357 | N   | THR | A | 183 | 32.373 | 17.112 | 28.207 | 1.00 | 29.62 | N |
| ATOM | 1358 | CA  | THR | A | 183 | 32.383 | 17.088 | 29.657 | 1.00 | 28.62 | C |
| ATOM | 1359 | C   | THR | A | 183 | 31.088 | 16.509 | 30.123 | 1.00 | 28.48 | C |
| ATOM | 1360 | O   | THR | A | 183 | 31.034 | 15.991 | 31.207 | 1.00 | 28.46 | O |
| ATOM | 1361 | CB  | THR | A | 183 | 32.504 | 18.509 | 30.276 | 1.00 | 28.82 | C |
| ATOM | 1362 | OG1 | THR | A | 183 | 31.441 | 19.364 | 29.795 | 1.00 | 28.93 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1363 | CG2 | THR | A | 183 | 33.764 | 19.178 | 29.846 | 1.00 | 28.28 | C |
| ATOM | 1364 | N   | SER | A | 184 | 30.005 | 16.673 | 29.355 | 1.00 | 28.14 | N |
| ATOM | 1365 | CA  | SER | A | 184 | 28.734 | 16.144 | 29.805 | 1.00 | 28.16 | C |
| ATOM | 1366 | C   | SER | A | 184 | 27.602 | 16.374 | 28.878 | 1.00 | 28.07 | C |
| ATOM | 1367 | O   | SER | A | 184 | 27.703 | 17.120 | 27.931 | 1.00 | 29.72 | O |
| ATOM | 1368 | CB  | SER | A | 184 | 28.357 | 16.750 | 31.149 | 1.00 | 27.81 | C |
| ATOM | 1369 | OG  | SER | A | 184 | 28.166 | 18.132 | 31.017 | 1.00 | 30.35 | O |
| ATOM | 1370 | N   | ASN | A | 185 | 26.505 | 15.721 | 29.176 | 1.00 | 27.93 | N |
| ATOM | 1371 | CA  | ASN | A | 185 | 25.288 | 15.850 | 28.434 | 1.00 | 28.66 | C |
| ATOM | 1372 | C   | ASN | A | 185 | 24.235 | 16.086 | 29.476 | 1.00 | 28.67 | C |
| ATOM | 1373 | O   | ASN | A | 185 | 23.974 | 15.226 | 30.291 | 1.00 | 27.67 | O |
| ATOM | 1374 | CB  | ASN | A | 185 | 24.927 | 14.543 | 27.683 | 1.00 | 28.53 | C |
| ATOM | 1375 | CG  | ASN | A | 185 | 25.914 | 14.191 | 26.589 | 1.00 | 29.19 | C |
| ATOM | 1376 | OD1 | ASN | A | 185 | 26.684 | 13.278 | 26.766 | 1.00 | 30.93 | O |
| ATOM | 1377 | ND2 | ASN | A | 185 | 25.891 | 14.910 | 25.451 | 1.00 | 29.67 | N |
| ATOM | 1378 | N   | LEU | A | 186 | 23.583 | 17.221 | 29.415 | 1.00 | 29.39 | N |
| ATOM | 1379 | CA  | LEU | A | 186 | 22.557 | 17.526 | 30.388 | 1.00 | 30.47 | C |
| ATOM | 1380 | C   | LEU | A | 186 | 21.179 | 17.177 | 29.835 | 1.00 | 30.85 | C |
| ATOM | 1381 | O   | LEU | A | 186 | 20.796 | 17.566 | 28.714 | 1.00 | 30.64 | O |
| ATOM | 1382 | CB  | LEU | A | 186 | 22.617 | 18.998 | 30.730 | 1.00 | 30.48 | C |
| ATOM | 1383 | CG  | LEU | A | 186 | 21.779 | 19.484 | 31.917 | 1.00 | 32.51 | C |
| ATOM | 1384 | CD1 | LEU | A | 186 | 22.330 | 18.952 | 33.238 | 1.00 | 31.55 | C |
| ATOM | 1385 | CD2 | LEU | A | 186 | 21.678 | 21.072 | 31.954 | 1.00 | 29.96 | C |
| ATOM | 1386 | N   | LEU | A | 187 | 20.409 | 16.439 | 30.613 | 1.00 | 31.21 | N |
| ATOM | 1387 | CA  | LEU | A | 187 | 19.042 | 16.155 | 30.188 | 1.00 | 30.60 | C |
| ATOM | 1388 | C   | LEU | A | 187 | 18.162 | 17.256 | 30.787 | 1.00 | 30.79 | C |
| ATOM | 1389 | O   | LEU | A | 187 | 18.257 | 17.557 | 31.991 | 1.00 | 29.69 | O |
| ATOM | 1390 | CB  | LEU | A | 187 | 18.626 | 14.781 | 30.644 | 1.00 | 30.50 | C |
| ATOM | 1391 | CG  | LEU | A | 187 | 17.130 | 14.465 | 30.590 | 1.00 | 32.29 | C |
| ATOM | 1392 | CD1 | LEU | A | 187 | 16.592 | 14.409 | 29.164 | 1.00 | 33.95 | C |
| ATOM | 1393 | CD2 | LEU | A | 187 | 16.864 | 13.137 | 31.270 | 1.00 | 32.62 | C |
| ATOM | 1394 | N   | LEU | A | 188 | 17.390 | 17.933 | 29.939 | 1.00 | 30.75 | N |
| ATOM | 1395 | CA  | LEU | A | 188 | 16.513 | 18.973 | 30.426 | 1.00 | 31.42 | C |
| ATOM | 1396 | C   | LEU | A | 188 | 15.053 | 18.646 | 30.107 | 1.00 | 32.02 | C |
| ATOM | 1397 | O   | LEU | A | 188 | 14.676 | 18.481 | 28.941 | 1.00 | 31.44 | O |
| ATOM | 1398 | CB  | LEU | A | 188 | 16.856 | 20.323 | 29.821 | 1.00 | 31.69 | C |
| ATOM | 1399 | CG  | LEU | A | 188 | 18.253 | 20.823 | 30.131 | 1.00 | 32.24 | C |
| ATOM | 1400 | CD1 | LEU | A | 188 | 19.094 | 20.883 | 28.904 | 1.00 | 32.79 | C |
| ATOM | 1401 | CD2 | LEU | A | 188 | 18.121 | 22.200 | 30.658 | 1.00 | 32.69 | C |
| ATOM | 1402 | N   | ILE | A | 189 | 14.228 | 18.568 | 31.146 | 1.00 | 32.26 | N |
| ATOM | 1403 | CA  | ILE | A | 189 | 12.816 | 18.305 | 30.944 | 1.00 | 32.23 | C |
| ATOM | 1404 | C   | ILE | A | 189 | 12.067 | 19.386 | 31.664 | 1.00 | 32.02 | C |
| ATOM | 1405 | O   | ILE | A | 189 | 12.194 | 19.520 | 32.895 | 1.00 | 31.42 | O |
| ATOM | 1406 | CB  | ILE | A | 189 | 12.427 | 16.966 | 31.479 | 1.00 | 32.05 | C |
| ATOM | 1407 | CG1 | ILE | A | 189 | 13.256 | 15.894 | 30.793 | 1.00 | 33.02 | C |
| ATOM | 1408 | CG2 | ILE | A | 189 | 10.957 | 16.764 | 31.232 | 1.00 | 32.90 | C |
| ATOM | 1409 | CD1 | ILE | A | 189 | 13.006 | 14.466 | 31.277 | 1.00 | 34.20 | C |
| ATOM | 1410 | N   | GLY | A | 190 | 11.279 | 20.145 | 30.898 | 1.00 | 31.94 | N |
| ATOM | 1411 | CA  | GLY | A | 190 | 10.623 | 21.334 | 31.414 | 1.00 | 31.49 | C |
| ATOM | 1412 | C   | GLY | A | 190 | 9.147  | 21.362 | 31.125 | 1.00 | 31.41 | C |
| ATOM | 1413 | O   | GLY | A | 190 | 8.671  | 20.649 | 30.245 | 1.00 | 30.40 | O |
| ATOM | 1414 | N   | MET | A | 191 | 8.433  | 22.154 | 31.914 | 1.00 | 31.55 | N |
| ATOM | 1415 | CA  | MET | A | 191 | 7.027  | 22.378 | 31.697 | 1.00 | 32.41 | C |
| ATOM | 1416 | C   | MET | A | 191 | 6.863  | 23.547 | 30.751 | 1.00 | 32.03 | C |
| ATOM | 1417 | O   | MET | A | 191 | 7.722  | 24.435 | 30.658 | 1.00 | 32.29 | O |
| ATOM | 1418 | CB  | MET | A | 191 | 6.313  | 22.672 | 33.008 | 1.00 | 33.21 | C |
| ATOM | 1419 | CG  | MET | A | 191 | 6.294  | 21.499 | 33.957 | 1.00 | 35.09 | C |
| ATOM | 1420 | SD  | MET | A | 191 | 5.828  | 21.953 | 35.652 | 1.00 | 39.51 | S |
| ATOM | 1421 | CE  | MET | A | 191 | 4.213  | 22.512 | 35.350 | 1.00 | 39.52 | C |
| ATOM | 1422 | N   | GLU | A | 192 | 5.755  | 23.539 | 30.033 | 1.00 | 31.96 | N |
| ATOM | 1423 | CA  | GLU | A | 192 | 5.459  | 24.588 | 29.081 | 1.00 | 32.31 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1424 | C   | GLU | A | 192 | 5.511  | 25.919 | 29.776 | 1.00 | 31.73 | C |
| ATOM | 1425 | O   | GLU | A | 192 | 5.096  | 26.041 | 30.913 | 1.00 | 31.73 | O |
| ATOM | 1426 | CB  | GLU | A | 192 | 4.087  | 24.375 | 28.508 | 1.00 | 33.09 | C |
| ATOM | 1427 | CG  | GLU | A | 192 | 2.995  | 24.434 | 29.552 | 1.00 | 34.74 | C |
| ATOM | 1428 | CD  | GLU | A | 192 | 1.679  | 23.940 | 29.019 | 1.00 | 36.73 | C |
| ATOM | 1429 | OE1 | GLU | A | 192 | 1.630  | 23.515 | 27.832 | 1.00 | 37.30 | O |
| ATOM | 1430 | OE2 | GLU | A | 192 | 0.698  | 24.001 | 29.791 | 1.00 | 38.64 | O |
| ATOM | 1431 | N   | GLY | A | 193 | 6.049  | 26.926 | 29.103 | 1.00 | 31.79 | N |
| ATOM | 1432 | CA  | GLY | A | 193 | 6.201  | 28.242 | 29.714 | 1.00 | 30.87 | C |
| ATOM | 1433 | C   | GLY | A | 193 | 7.480  | 28.432 | 30.521 | 1.00 | 30.28 | C |
| ATOM | 1434 | O   | GLY | A | 193 | 7.777  | 29.534 | 30.901 | 1.00 | 30.29 | O |
| ATOM | 1435 | N   | ASN | A | 194 | 8.223  | 27.375 | 30.825 | 1.00 | 29.85 | N |
| ATOM | 1436 | CA  | ASN | A | 194 | 9.460  | 27.536 | 31.604 | 1.00 | 29.38 | C |
| ATOM | 1437 | C   | ASN | A | 194 | 10.473 | 28.371 | 30.840 | 1.00 | 28.61 | C |
| ATOM | 1438 | O   | ASN | A | 194 | 10.606 | 28.216 | 29.615 | 1.00 | 28.58 | O |
| ATOM | 1439 | CB  | ASN | A | 194 | 10.136 | 26.186 | 31.866 | 1.00 | 29.15 | C |
| ATOM | 1440 | CG  | ASN | A | 194 | 9.565  | 25.445 | 33.049 | 1.00 | 29.50 | C |
| ATOM | 1441 | OD1 | ASN | A | 194 | 8.632  | 25.896 | 33.714 | 1.00 | 32.61 | O |
| ATOM | 1442 | ND2 | ASN | A | 194 | 10.146 | 24.305 | 33.334 | 1.00 | 28.53 | N |
| ATOM | 1443 | N   | VAL | A | 195 | 11.221 | 29.194 | 31.561 | 1.00 | 27.70 | N |
| ATOM | 1444 | CA  | VAL | A | 195 | 12.272 | 29.998 | 30.962 | 1.00 | 27.80 | C |
| ATOM | 1445 | C   | VAL | A | 195 | 13.586 | 29.858 | 31.701 | 1.00 | 27.07 | C |
| ATOM | 1446 | O   | VAL | A | 195 | 13.636 | 29.898 | 32.939 | 1.00 | 27.43 | O |
| ATOM | 1447 | CB  | VAL | A | 195 | 11.904 | 31.520 | 31.018 | 1.00 | 28.18 | C |
| ATOM | 1448 | CG1 | VAL | A | 195 | 13.056 | 32.371 | 30.560 | 1.00 | 26.78 | C |
| ATOM | 1449 | CG2 | VAL | A | 195 | 10.662 | 31.789 | 30.187 | 1.00 | 29.06 | C |
| ATOM | 1450 | N   | THR | A | 196 | 14.659 | 29.712 | 30.953 | 1.00 | 26.48 | N |
| ATOM | 1451 | CA  | THR | A | 196 | 15.994 | 29.811 | 31.530 | 1.00 | 26.08 | C |
| ATOM | 1452 | C   | THR | A | 196 | 16.462 | 31.184 | 31.084 | 1.00 | 27.03 | C |
| ATOM | 1453 | O   | THR | A | 196 | 16.614 | 31.425 | 29.876 | 1.00 | 26.51 | O |
| ATOM | 1454 | CB  | THR | A | 196 | 16.915 | 28.811 | 30.934 | 1.00 | 25.96 | C |
| ATOM | 1455 | OG1 | THR | A | 196 | 16.525 | 27.478 | 31.309 | 1.00 | 26.20 | O |
| ATOM | 1456 | CG2 | THR | A | 196 | 18.340 | 29.012 | 31.457 | 1.00 | 23.99 | C |
| ATOM | 1457 | N   | PRO | A | 197 | 16.647 | 32.090 | 32.036 | 1.00 | 27.21 | N |
| ATOM | 1458 | CA  | PRO | A | 197 | 17.053 | 33.451 | 31.725 | 1.00 | 27.46 | C |
| ATOM | 1459 | C   | PRO | A | 197 | 18.432 | 33.512 | 31.113 | 1.00 | 27.48 | C |
| ATOM | 1460 | O   | PRO | A | 197 | 19.248 | 32.588 | 31.293 | 1.00 | 27.52 | O |
| ATOM | 1461 | CB  | PRO | A | 197 | 17.007 | 34.166 | 33.075 | 1.00 | 27.56 | C |
| ATOM | 1462 | CG  | PRO | A | 197 | 16.226 | 33.344 | 33.924 | 1.00 | 28.15 | C |
| ATOM | 1463 | CD  | PRO | A | 197 | 16.384 | 31.914 | 33.470 | 1.00 | 27.92 | C |
| ATOM | 1464 | N   | ALA | A | 198 | 18.668 | 34.616 | 30.413 | 1.00 | 26.77 | N |
| ATOM | 1465 | CA  | ALA | A | 198 | 19.877 | 34.830 | 29.647 | 1.00 | 26.92 | C |
| ATOM | 1466 | C   | ALA | A | 198 | 21.172 | 34.681 | 30.438 | 1.00 | 27.14 | C |
| ATOM | 1467 | O   | ALA | A | 198 | 21.354 | 35.278 | 31.520 | 1.00 | 25.53 | O |
| ATOM | 1468 | CB  | ALA | A | 198 | 19.828 | 36.235 | 29.021 | 1.00 | 27.07 | C |
| ATOM | 1469 | N   | HIS | A | 199 | 22.091 | 33.929 | 29.839 | 1.00 | 27.28 | N |
| ATOM | 1470 | CA  | HIS | A | 199 | 23.399 | 33.673 | 30.424 | 1.00 | 27.81 | C |
| ATOM | 1471 | C   | HIS | A | 199 | 24.319 | 33.208 | 29.333 | 1.00 | 28.09 | C |
| ATOM | 1472 | O   | HIS | A | 199 | 23.857 | 32.933 | 28.197 | 1.00 | 28.34 | O |
| ATOM | 1473 | CB  | HIS | A | 199 | 23.323 | 32.549 | 31.461 | 1.00 | 27.10 | C |
| ATOM | 1474 | CG  | HIS | A | 199 | 22.963 | 31.221 | 30.864 | 1.00 | 29.70 | C |
| ATOM | 1475 | ND1 | HIS | A | 199 | 21.668 | 30.891 | 30.525 | 1.00 | 30.01 | N |
| ATOM | 1476 | CD2 | HIS | A | 199 | 23.728 | 30.180 | 30.463 | 1.00 | 29.60 | C |
| ATOM | 1477 | CE1 | HIS | A | 199 | 21.647 | 29.684 | 29.993 | 1.00 | 29.66 | C |
| ATOM | 1478 | NE2 | HIS | A | 199 | 22.881 | 29.236 | 29.926 | 1.00 | 30.43 | N |
| ATOM | 1479 | N   | TYR | A | 200 | 25.612 | 33.104 | 29.671 | 1.00 | 28.30 | N |
| ATOM | 1480 | CA  | TYR | A | 200 | 26.607 | 32.518 | 28.769 | 1.00 | 28.15 | C |
| ATOM | 1481 | C   | TYR | A | 200 | 27.298 | 31.351 | 29.482 | 1.00 | 27.91 | C |
| ATOM | 1482 | O   | TYR | A | 200 | 27.335 | 31.333 | 30.690 | 1.00 | 27.87 | O |
| ATOM | 1483 | CB  | TYR | A | 200 | 27.585 | 33.534 | 28.217 | 1.00 | 28.02 | C |
| ATOM | 1484 | CG  | TYR | A | 200 | 28.540 | 34.142 | 29.226 | 1.00 | 29.58 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1485 | CD1 | TYR | A | 200 | 29.784 | 33.571 | 29.462 | 1.00 | 28.14 | C |
| ATOM | 1486 | CD2 | TYR | A | 200 | 28.231 | 35.342 | 29.871 | 1.00 | 29.32 | C |
| ATOM | 1487 | CE1 | TYR | A | 200 | 30.660 | 34.128 | 30.367 | 1.00 | 30.20 | C |
| ATOM | 1488 | CE2 | TYR | A | 200 | 29.107 | 35.919 | 30.777 | 1.00 | 29.61 | C |
| ATOM | 1489 | CZ  | TYR | A | 200 | 30.319 | 35.315 | 31.031 | 1.00 | 29.78 | C |
| ATOM | 1490 | OH  | TYR | A | 200 | 31.180 | 35.864 | 31.940 | 1.00 | 24.43 | O |
| ATOM | 1491 | N   | ASP | A | 201 | 27.797 | 30.363 | 28.727 | 1.00 | 27.73 | N |
| ATOM | 1492 | CA  | ASP | A | 201 | 28.461 | 29.180 | 29.302 | 1.00 | 27.65 | C |
| ATOM | 1493 | C   | ASP | A | 201 | 29.873 | 29.220 | 28.799 | 1.00 | 27.87 | C |
| ATOM | 1494 | O   | ASP | A | 201 | 30.080 | 29.765 | 27.768 | 1.00 | 27.68 | O |
| ATOM | 1495 | CB  | ASP | A | 201 | 27.775 | 27.884 | 28.855 | 1.00 | 26.32 | C |
| ATOM | 1496 | CG  | ASP | A | 201 | 26.356 | 27.768 | 29.363 | 1.00 | 25.12 | C |
| ATOM | 1497 | OD1 | ASP | A | 201 | 26.156 | 27.722 | 30.605 | 1.00 | 23.49 | O |
| ATOM | 1498 | OD2 | ASP | A | 201 | 25.360 | 27.687 | 28.589 | 1.00 | 27.18 | O |
| ATOM | 1499 | N   | GLU | A | 202 | 30.843 | 28.682 | 29.520 | 1.00 | 29.28 | N |
| ATOM | 1500 | CA  | GLU | A | 202 | 32.228 | 28.672 | 29.013 | 1.00 | 31.18 | C |
| ATOM | 1501 | C   | GLU | A | 202 | 32.571 | 27.435 | 28.190 | 1.00 | 31.54 | C |
| ATOM | 1502 | O   | GLU | A | 202 | 33.734 | 27.060 | 28.139 | 1.00 | 33.48 | O |
| ATOM | 1503 | CB  | GLU | A | 202 | 33.250 | 28.741 | 30.155 | 1.00 | 30.78 | C |
| ATOM | 1504 | CG  | GLU | A | 202 | 33.122 | 29.981 | 31.003 | 1.00 | 33.61 | C |
| ATOM | 1505 | CD  | GLU | A | 202 | 34.194 | 30.081 | 32.062 | 1.00 | 35.96 | C |
| ATOM | 1506 | OE1 | GLU | A | 202 | 34.036 | 29.531 | 33.166 | 1.00 | 41.25 | O |
| ATOM | 1507 | OE2 | GLU | A | 202 | 35.199 | 30.718 | 31.788 | 1.00 | 39.13 | O |
| ATOM | 1508 | N   | GLN | A | 203 | 31.582 | 26.747 | 27.641 | 1.00 | 31.19 | N |
| ATOM | 1509 | CA  | GLN | A | 203 | 31.844 | 25.589 | 26.833 | 1.00 | 30.78 | C |
| ATOM | 1510 | C   | GLN | A | 203 | 31.078 | 25.743 | 25.556 | 1.00 | 29.96 | C |
| ATOM | 1511 | O   | GLN | A | 203 | 30.213 | 26.581 | 25.462 | 1.00 | 30.22 | O |
| ATOM | 1512 | CB  | GLN | A | 203 | 31.427 | 24.315 | 27.546 | 1.00 | 31.32 | C |
| ATOM | 1513 | CG  | GLN | A | 203 | 32.364 | 23.971 | 28.725 | 1.00 | 34.97 | C |
| ATOM | 1514 | CD  | GLN | A | 203 | 32.204 | 22.548 | 29.288 | 1.00 | 35.23 | C |
| ATOM | 1515 | OE1 | GLN | A | 203 | 32.161 | 21.559 | 28.551 | 1.00 | 36.82 | O |
| ATOM | 1516 | NE2 | GLN | A | 203 | 32.160 | 22.456 | 30.600 | 1.00 | 35.56 | N |
| ATOM | 1517 | N   | GLN | A | 204 | 31.461 | 24.961 | 24.555 | 1.00 | 29.46 | N |
| ATOM | 1518 | CA  | GLN | A | 204 | 30.791 | 24.911 | 23.292 | 1.00 | 28.65 | C |
| ATOM | 1519 | C   | GLN | A | 204 | 29.641 | 23.941 | 23.494 | 1.00 | 28.27 | C |
| ATOM | 1520 | O   | GLN | A | 204 | 29.797 | 22.941 | 24.194 | 1.00 | 27.65 | O |
| ATOM | 1521 | CB  | GLN | A | 204 | 31.717 | 24.381 | 22.214 | 1.00 | 29.02 | C |
| ATOM | 1522 | CG  | GLN | A | 204 | 33.006 | 25.154 | 22.028 | 1.00 | 28.50 | C |
| ATOM | 1523 | CD  | GLN | A | 204 | 32.818 | 26.366 | 21.150 | 1.00 | 27.16 | C |
| ATOM | 1524 | OE1 | GLN | A | 204 | 31.690 | 26.742 | 20.846 | 1.00 | 22.90 | O |
| ATOM | 1525 | NE2 | GLN | A | 204 | 33.921 | 26.952 | 20.714 | 1.00 | 23.20 | N |
| ATOM | 1526 | N   | ASN | A | 205 | 28.497 | 24.219 | 22.864 | 1.00 | 27.36 | N |
| ATOM | 1527 | CA  | ASN | A | 205 | 27.302 | 23.424 | 23.058 | 1.00 | 27.13 | C |
| ATOM | 1528 | C   | ASN | A | 205 | 26.552 | 23.052 | 21.777 | 1.00 | 27.39 | C |
| ATOM | 1529 | O   | ASN | A | 205 | 26.151 | 23.930 | 20.999 | 1.00 | 27.36 | O |
| ATOM | 1530 | CB  | ASN | A | 205 | 26.378 | 24.229 | 23.967 | 1.00 | 26.95 | C |
| ATOM | 1531 | CG  | ASN | A | 205 | 25.083 | 23.525 | 24.327 | 1.00 | 27.30 | C |
| ATOM | 1532 | OD1 | ASN | A | 205 | 24.726 | 22.453 | 23.818 | 1.00 | 27.11 | O |
| ATOM | 1533 | ND2 | ASN | A | 205 | 24.319 | 24.190 | 25.171 | 1.00 | 24.64 | N |
| ATOM | 1534 | N   | PHE | A | 206 | 26.383 | 21.749 | 21.542 | 1.00 | 26.46 | N |
| ATOM | 1535 | CA  | PHE | A | 206 | 25.417 | 21.334 | 20.554 | 1.00 | 25.88 | C |
| ATOM | 1536 | C   | PHE | A | 206 | 24.181 | 20.946 | 21.373 | 1.00 | 25.65 | C |
| ATOM | 1537 | O   | PHE | A | 206 | 24.230 | 19.988 | 22.178 | 1.00 | 25.16 | O |
| ATOM | 1538 | CB  | PHE | A | 206 | 25.909 | 20.170 | 19.717 | 1.00 | 26.28 | C |
| ATOM | 1539 | CG  | PHE | A | 206 | 26.837 | 20.566 | 18.636 | 1.00 | 24.81 | C |
| ATOM | 1540 | CD1 | PHE | A | 206 | 26.416 | 21.374 | 17.633 | 1.00 | 26.27 | C |
| ATOM | 1541 | CD2 | PHE | A | 206 | 28.122 | 20.098 | 18.616 | 1.00 | 25.53 | C |
| ATOM | 1542 | CE1 | PHE | A | 206 | 27.248 | 21.736 | 16.634 | 1.00 | 27.05 | C |
| ATOM | 1543 | CE2 | PHE | A | 206 | 28.991 | 20.469 | 17.617 | 1.00 | 26.80 | C |
| ATOM | 1544 | CZ  | PHE | A | 206 | 28.549 | 21.274 | 16.619 | 1.00 | 28.34 | C |
| ATOM | 1545 | N   | PHE | A | 207 | 23.084 | 21.648 | 21.086 | 1.00 | 25.08 | N |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1546 | CA  | PHE | A | 207 | 21.809 | 21.625 | 21.827 | 1.00 | 25.52 | C |
| ATOM | 1547 | C   | PHE | A | 207 | 20.775 | 20.885 | 21.011 | 1.00 | 25.55 | C |
| ATOM | 1548 | O   | PHE | A | 207 | 20.261 | 21.410 | 20.058 | 1.00 | 25.61 | O |
| ATOM | 1549 | CB  | PHE | A | 207 | 21.408 | 23.107 | 22.074 | 1.00 | 25.37 | C |
| ATOM | 1550 | CG  | PHE | A | 207 | 20.146 | 23.346 | 22.872 | 1.00 | 23.70 | C |
| ATOM | 1551 | CD1 | PHE | A | 207 | 18.938 | 23.547 | 22.234 | 1.00 | 24.08 | C |
| ATOM | 1552 | CD2 | PHE | A | 207 | 20.199 | 23.551 | 24.220 | 1.00 | 25.24 | C |
| ATOM | 1553 | CE1 | PHE | A | 207 | 17.800 | 23.864 | 22.927 | 1.00 | 24.50 | C |
| ATOM | 1554 | CE2 | PHE | A | 207 | 19.035 | 23.883 | 24.959 | 1.00 | 26.04 | C |
| ATOM | 1555 | CZ  | PHE | A | 207 | 17.836 | 24.021 | 24.298 | 1.00 | 26.68 | C |
| ATOM | 1556 | N   | ALA | A | 208 | 20.490 | 19.657 | 21.422 | 1.00 | 26.60 | N |
| ATOM | 1557 | CA  | ALA | A | 208 | 19.667 | 18.710 | 20.689 | 1.00 | 26.45 | C |
| ATOM | 1558 | C   | ALA | A | 208 | 18.231 | 18.594 | 21.210 | 1.00 | 27.10 | C |
| ATOM | 1559 | O   | ALA | A | 208 | 17.966 | 17.987 | 22.273 | 1.00 | 26.47 | O |
| ATOM | 1560 | CB  | ALA | A | 208 | 20.303 | 17.363 | 20.766 | 1.00 | 25.67 | C |
| ATOM | 1561 | N   | GLN | A | 209 | 17.306 | 19.121 | 20.419 | 1.00 | 27.02 | N |
| ATOM | 1562 | CA  | GLN | A | 209 | 15.918 | 19.125 | 20.833 | 1.00 | 27.37 | C |
| ATOM | 1563 | C   | GLN | A | 209 | 15.276 | 17.781 | 20.519 | 1.00 | 27.55 | C |
| ATOM | 1564 | O   | GLN | A | 209 | 15.489 | 17.190 | 19.427 | 1.00 | 26.51 | O |
| ATOM | 1565 | CB  | GLN | A | 209 | 15.195 | 20.301 | 20.179 | 1.00 | 27.15 | C |
| ATOM | 1566 | CG  | GLN | A | 209 | 13.806 | 20.508 | 20.662 | 1.00 | 27.77 | C |
| ATOM | 1567 | CD  | GLN | A | 209 | 13.740 | 20.959 | 22.126 | 1.00 | 29.40 | C |
| ATOM | 1568 | OE1 | GLN | A | 209 | 14.773 | 21.166 | 22.774 | 1.00 | 27.27 | O |
| ATOM | 1569 | NE2 | GLN | A | 209 | 12.517 | 21.118 | 22.636 | 1.00 | 27.15 | N |
| ATOM | 1570 | N   | ILE | A | 210 | 14.461 | 17.327 | 21.473 | 1.00 | 28.32 | N |
| ATOM | 1571 | CA  | ILE | A | 210 | 13.897 | 15.998 | 21.429 | 1.00 | 29.37 | C |
| ATOM | 1572 | C   | ILE | A | 210 | 12.403 | 15.966 | 21.435 | 1.00 | 30.37 | C |
| ATOM | 1573 | O   | ILE | A | 210 | 11.849 | 15.275 | 20.619 | 1.00 | 31.58 | O |
| ATOM | 1574 | CB  | ILE | A | 210 | 14.413 | 15.204 | 22.605 | 1.00 | 29.80 | C |
| ATOM | 1575 | CG1 | ILE | A | 210 | 15.830 | 14.734 | 22.302 | 1.00 | 30.27 | C |
| ATOM | 1576 | CG2 | ILE | A | 210 | 13.525 | 14.005 | 22.864 | 1.00 | 30.25 | C |
| ATOM | 1577 | CD1 | ILE | A | 210 | 16.624 | 14.421 | 23.516 | 1.00 | 32.28 | C |
| ATOM | 1578 | N   | LYS | A | 211 | 11.757 | 16.664 | 22.374 | 1.00 | 31.18 | N |
| ATOM | 1579 | CA  | LYS | A | 211 | 10.300 | 16.723 | 22.438 | 1.00 | 31.16 | C |
| ATOM | 1580 | C   | LYS | A | 211 | 9.887  | 18.137 | 22.706 | 1.00 | 31.19 | C |
| ATOM | 1581 | O   | LYS | A | 211 | 10.495 | 18.800 | 23.523 | 1.00 | 31.21 | O |
| ATOM | 1582 | CB  | LYS | A | 211 | 9.767  | 15.891 | 23.591 | 1.00 | 32.00 | C |
| ATOM | 1583 | CG  | LYS | A | 211 | 8.240  | 15.758 | 23.629 | 1.00 | 32.36 | C |
| ATOM | 1584 | CD  | LYS | A | 211 | 7.787  | 15.177 | 24.970 | 1.00 | 33.23 | C |
| ATOM | 1585 | CE  | LYS | A | 211 | 6.497  | 14.368 | 24.883 | 1.00 | 35.14 | C |
| ATOM | 1586 | NZ  | LYS | A | 211 | 5.506  | 14.755 | 23.835 | 1.00 | 35.43 | N |
| ATOM | 1587 | N   | GLY | A | 212 | 8.844  | 18.592 | 22.018 | 1.00 | 31.20 | N |
| ATOM | 1588 | CA  | GLY | A | 212 | 8.337  | 19.934 | 22.174 | 1.00 | 30.96 | C |
| ATOM | 1589 | C   | GLY | A | 212 | 9.209  | 20.975 | 21.495 | 1.00 | 31.42 | C |
| ATOM | 1590 | O   | GLY | A | 212 | 10.167 | 20.670 | 20.771 | 1.00 | 31.06 | O |
| ATOM | 1591 | N   | TYR | A | 213 | 8.857  | 22.224 | 21.734 | 1.00 | 31.43 | N |
| ATOM | 1592 | CA  | TYR | A | 213 | 9.507  | 23.319 | 21.057 | 1.00 | 31.80 | C |
| ATOM | 1593 | C   | TYR | A | 213 | 10.046 | 24.332 | 22.043 | 1.00 | 31.00 | C |
| ATOM | 1594 | O   | TYR | A | 213 | 9.411  | 24.649 | 23.038 | 1.00 | 29.31 | O |
| ATOM | 1595 | CB  | TYR | A | 213 | 8.502  | 23.959 | 20.127 | 1.00 | 32.64 | C |
| ATOM | 1596 | CG  | TYR | A | 213 | 8.103  | 23.039 | 19.015 | 1.00 | 35.60 | C |
| ATOM | 1597 | CD1 | TYR | A | 213 | 7.089  | 22.071 | 19.174 | 1.00 | 38.37 | C |
| ATOM | 1598 | CD2 | TYR | A | 213 | 8.758  | 23.110 | 17.813 | 1.00 | 37.73 | C |
| ATOM | 1599 | CE1 | TYR | A | 213 | 6.765  | 21.223 | 18.137 | 1.00 | 39.37 | C |
| ATOM | 1600 | CE2 | TYR | A | 213 | 8.443  | 22.292 | 16.792 | 1.00 | 39.75 | C |
| ATOM | 1601 | CZ  | TYR | A | 213 | 7.460  | 21.364 | 16.924 | 1.00 | 41.66 | C |
| ATOM | 1602 | OH  | TYR | A | 213 | 7.232  | 20.603 | 15.782 | 1.00 | 46.53 | O |
| ATOM | 1603 | N   | LYS | A | 214 | 11.260 | 24.787 | 21.777 | 1.00 | 30.99 | N |
| ATOM | 1604 | CA  | LYS | A | 214 | 11.886 | 25.804 | 22.594 | 1.00 | 31.15 | C |
| ATOM | 1605 | C   | LYS | A | 214 | 12.305 | 26.993 | 21.762 | 1.00 | 31.00 | C |
| ATOM | 1606 | O   | LYS | A | 214 | 12.914 | 26.838 | 20.695 | 1.00 | 31.84 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1607 | CB  | LYS | A | 214 | 13.112 | 25.244 | 23.311 | 1.00 | 31.08 | C |
| ATOM | 1608 | CG  | LYS | A | 214 | 12.806 | 24.432 | 24.557 | 1.00 | 30.96 | C |
| ATOM | 1609 | CD  | LYS | A | 214 | 14.106 | 23.949 | 25.159 | 1.00 | 30.84 | C |
| ATOM | 1610 | CE  | LYS | A | 214 | 13.982 | 23.555 | 26.584 | 1.00 | 29.59 | C |
| ATOM | 1611 | NZ  | LYS | A | 214 | 15.278 | 23.118 | 27.162 | 1.00 | 28.16 | N |
| ATOM | 1612 | N   | ARG | A | 215 | 11.992 | 28.193 | 22.241 | 1.00 | 30.59 | N |
| ATOM | 1613 | CA  | ARG | A | 215 | 12.445 | 29.385 | 21.549 | 1.00 | 29.98 | C |
| ATOM | 1614 | C   | ARG | A | 215 | 13.764 | 29.790 | 22.154 | 1.00 | 29.65 | C |
| ATOM | 1615 | O   | ARG | A | 215 | 13.850 | 29.982 | 23.349 | 1.00 | 29.61 | O |
| ATOM | 1616 | CB  | ARG | A | 215 | 11.431 | 30.502 | 21.690 | 1.00 | 30.08 | C |
| ATOM | 1617 | CG  | ARG | A | 215 | 11.835 | 31.810 | 21.004 | 1.00 | 29.82 | C |
| ATOM | 1618 | CD  | ARG | A | 215 | 11.221 | 32.960 | 21.731 | 1.00 | 32.78 | C |
| ATOM | 1619 | NE  | ARG | A | 215 | 11.211 | 34.189 | 20.975 | 1.00 | 33.81 | N |
| ATOM | 1620 | CZ  | ARG | A | 215 | 10.540 | 35.259 | 21.336 | 1.00 | 35.12 | C |
| ATOM | 1621 | NH1 | ARG | A | 215 | 9.828  | 35.262 | 22.441 | 1.00 | 35.28 | N |
| ATOM | 1622 | NH2 | ARG | A | 215 | 10.586 | 36.338 | 20.581 | 1.00 | 39.28 | N |
| ATOM | 1623 | N   | CYS | A | 216 | 14.791 | 29.909 | 21.327 | 1.00 | 29.86 | N |
| ATOM | 1624 | CA  | CYS | A | 216 | 16.129 | 30.237 | 21.797 | 1.00 | 29.64 | C |
| ATOM | 1625 | C   | CYS | A | 216 | 16.533 | 31.603 | 21.274 | 1.00 | 30.06 | C |
| ATOM | 1626 | O   | CYS | A | 216 | 16.516 | 31.807 | 20.092 | 1.00 | 31.32 | O |
| ATOM | 1627 | CB  | CYS | A | 216 | 17.113 | 29.183 | 21.275 | 1.00 | 29.78 | C |
| ATOM | 1628 | SG  | CYS | A | 216 | 16.658 | 27.438 | 21.641 | 1.00 | 30.35 | S |
| ATOM | 1629 | N   | ILE | A | 217 | 16.849 | 32.556 | 22.149 | 1.00 | 30.28 | N |
| ATOM | 1630 | CA  | ILE | A | 217 | 17.303 | 33.876 | 21.744 | 1.00 | 29.78 | C |
| ATOM | 1631 | C   | ILE | A | 217 | 18.758 | 34.017 | 22.203 | 1.00 | 29.42 | C |
| ATOM | 1632 | O   | ILE | A | 217 | 19.050 | 33.852 | 23.385 | 1.00 | 28.77 | O |
| ATOM | 1633 | CB  | ILE | A | 217 | 16.427 | 34.969 | 22.391 | 1.00 | 30.51 | C |
| ATOM | 1634 | CG1 | ILE | A | 217 | 14.934 | 34.705 | 22.111 | 1.00 | 31.29 | C |
| ATOM | 1635 | CG2 | ILE | A | 217 | 16.785 | 36.313 | 21.843 | 1.00 | 30.11 | C |
| ATOM | 1636 | CD1 | ILE | A | 217 | 14.009 | 35.655 | 22.847 | 1.00 | 33.08 | C |
| ATOM | 1637 | N   | LEU | A | 218 | 19.647 | 34.326 | 21.257 | 1.00 | 28.60 | N |
| ATOM | 1638 | CA  | LEU | A | 218 | 21.059 | 34.392 | 21.501 | 1.00 | 28.59 | C |
| ATOM | 1639 | C   | LEU | A | 218 | 21.606 | 35.781 | 21.257 | 1.00 | 28.74 | C |
| ATOM | 1640 | O   | LEU | A | 218 | 21.102 | 36.522 | 20.412 | 1.00 | 29.64 | O |
| ATOM | 1641 | CB  | LEU | A | 218 | 21.788 | 33.422 | 20.574 | 1.00 | 28.52 | C |
| ATOM | 1642 | CG  | LEU | A | 218 | 21.927 | 31.980 | 21.028 | 1.00 | 28.46 | C |
| ATOM | 1643 | CD1 | LEU | A | 218 | 20.569 | 31.318 | 21.233 | 1.00 | 28.95 | C |
| ATOM | 1644 | CD2 | LEU | A | 218 | 22.707 | 31.196 | 20.026 | 1.00 | 27.94 | C |
| ATOM | 1645 | N   | PHE | A | 219 | 22.659 | 36.145 | 21.986 | 1.00 | 28.61 | N |
| ATOM | 1646 | CA  | PHE | A | 219 | 23.309 | 37.458 | 21.774 | 1.00 | 28.07 | C |
| ATOM | 1647 | C   | PHE | A | 219 | 24.811 | 37.221 | 21.710 | 1.00 | 28.25 | C |
| ATOM | 1648 | O   | PHE | A | 219 | 25.352 | 36.468 | 22.517 | 1.00 | 28.82 | O |
| ATOM | 1649 | CB  | PHE | A | 219 | 22.987 | 38.415 | 22.908 | 1.00 | 26.73 | C |
| ATOM | 1650 | CG  | PHE | A | 219 | 21.522 | 38.553 | 23.199 | 1.00 | 27.28 | C |
| ATOM | 1651 | CD1 | PHE | A | 219 | 20.874 | 37.658 | 24.029 | 1.00 | 25.73 | C |
| ATOM | 1652 | CD2 | PHE | A | 219 | 20.782 | 39.598 | 22.648 | 1.00 | 28.57 | C |
| ATOM | 1653 | CE1 | PHE | A | 219 | 19.536 | 37.811 | 24.311 | 1.00 | 26.59 | C |
| ATOM | 1654 | CE2 | PHE | A | 219 | 19.443 | 39.722 | 22.898 | 1.00 | 27.78 | C |
| ATOM | 1655 | CZ  | PHE | A | 219 | 18.816 | 38.828 | 23.725 | 1.00 | 28.22 | C |
| ATOM | 1656 | N   | PRO | A | 220 | 25.501 | 37.840 | 20.776 | 1.00 | 28.30 | N |
| ATOM | 1657 | CA  | PRO | A | 220 | 26.946 | 37.641 | 20.675 | 1.00 | 28.76 | C |
| ATOM | 1658 | C   | PRO | A | 220 | 27.688 | 38.195 | 21.881 | 1.00 | 29.07 | C |
| ATOM | 1659 | O   | PRO | A | 220 | 27.172 | 39.019 | 22.661 | 1.00 | 29.11 | O |
| ATOM | 1660 | CB  | PRO | A | 220 | 27.336 | 38.413 | 19.426 | 1.00 | 28.79 | C |
| ATOM | 1661 | CG  | PRO | A | 220 | 26.016 | 38.847 | 18.795 | 1.00 | 29.65 | C |
| ATOM | 1662 | CD  | PRO | A | 220 | 24.987 | 38.794 | 19.790 | 1.00 | 28.85 | C |
| ATOM | 1663 | N   | PRO | A | 221 | 28.914 | 37.727 | 22.057 | 1.00 | 29.09 | N |
| ATOM | 1664 | CA  | PRO | A | 221 | 29.725 | 38.147 | 23.188 | 1.00 | 28.85 | C |
| ATOM | 1665 | C   | PRO | A | 221 | 29.979 | 39.656 | 23.199 | 1.00 | 28.60 | C |
| ATOM | 1666 | O   | PRO | A | 221 | 30.223 | 40.182 | 24.270 | 1.00 | 26.85 | O |
| ATOM | 1667 | CB  | PRO | A | 221 | 31.018 | 37.412 | 22.975 | 1.00 | 29.01 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1668 | CG  | PRO | A | 221 | 30.665 | 36.286 | 22.114 | 1.00 | 30.46 | C |
| ATOM | 1669 | CD  | PRO | A | 221 | 29.580 | 36.722 | 21.232 | 1.00 | 29.52 | C |
| ATOM | 1670 | N   | ASP | A | 222 | 29.853 | 40.335 | 22.062 | 1.00 | 28.17 | N |
| ATOM | 1671 | CA  | ASP | A | 222 | 30.155 | 41.763 | 22.044 | 1.00 | 28.79 | C |
| ATOM | 1672 | C   | ASP | A | 222 | 28.976 | 42.554 | 22.533 | 1.00 | 28.84 | C |
| ATOM | 1673 | O   | ASP | A | 222 | 28.948 | 43.767 | 22.432 | 1.00 | 30.46 | O |
| ATOM | 1674 | CB  | ASP | A | 222 | 30.631 | 42.287 | 20.693 | 1.00 | 27.27 | C |
| ATOM | 1675 | CG  | ASP | A | 222 | 29.541 | 42.288 | 19.655 | 1.00 | 30.76 | C |
| ATOM | 1676 | OD1 | ASP | A | 222 | 28.368 | 41.926 | 19.920 | 1.00 | 30.56 | O |
| ATOM | 1677 | OD2 | ASP | A | 222 | 29.785 | 42.609 | 18.495 | 1.00 | 39.36 | O |
| ATOM | 1678 | N   | GLN | A | 223 | 28.000 | 41.885 | 23.083 | 1.00 | 29.33 | N |
| ATOM | 1679 | CA  | GLN | A | 223 | 26.902 | 42.614 | 23.676 | 1.00 | 29.61 | C |
| ATOM | 1680 | C   | GLN | A | 223 | 27.012 | 42.533 | 25.194 | 1.00 | 28.97 | C |
| ATOM | 1681 | O   | GLN | A | 223 | 26.065 | 42.825 | 25.919 | 1.00 | 29.82 | O |
| ATOM | 1682 | CB  | GLN | A | 223 | 25.575 | 42.131 | 23.110 | 1.00 | 30.22 | C |
| ATOM | 1683 | CG  | GLN | A | 223 | 25.244 | 42.854 | 21.762 | 1.00 | 33.01 | C |
| ATOM | 1684 | CD  | GLN | A | 223 | 23.866 | 42.562 | 21.241 | 1.00 | 37.71 | C |
| ATOM | 1685 | OE1 | GLN | A | 223 | 22.899 | 42.573 | 22.005 | 1.00 | 43.11 | O |
| ATOM | 1686 | NE2 | GLN | A | 223 | 23.760 | 42.285 | 19.943 | 1.00 | 38.91 | N |
| ATOM | 1687 | N   | PHE | A | 224 | 28.181 | 42.148 | 25.672 | 1.00 | 27.69 | N |
| ATOM | 1688 | CA  | PHE | A | 224 | 28.452 | 42.168 | 27.115 | 1.00 | 28.30 | C |
| ATOM | 1689 | C   | PHE | A | 224 | 27.932 | 43.497 | 27.771 | 1.00 | 29.27 | C |
| ATOM | 1690 | O   | PHE | A | 224 | 27.248 | 43.448 | 28.786 | 1.00 | 29.24 | O |
| ATOM | 1691 | CB  | PHE | A | 224 | 29.968 | 42.025 | 27.373 | 1.00 | 26.64 | C |
| ATOM | 1692 | CG  | PHE | A | 224 | 30.338 | 41.881 | 28.810 | 1.00 | 27.05 | C |
| ATOM | 1693 | CD1 | PHE | A | 224 | 30.526 | 42.992 | 29.619 | 1.00 | 26.91 | C |
| ATOM | 1694 | CD2 | PHE | A | 224 | 30.560 | 40.649 | 29.365 | 1.00 | 25.77 | C |
| ATOM | 1695 | CE1 | PHE | A | 224 | 30.878 | 42.864 | 30.930 | 1.00 | 24.95 | C |
| ATOM | 1696 | CE2 | PHE | A | 224 | 30.928 | 40.522 | 30.675 | 1.00 | 25.92 | C |
| ATOM | 1697 | CZ  | PHE | A | 224 | 31.056 | 41.641 | 31.467 | 1.00 | 27.45 | C |
| ATOM | 1698 | N   | GLU | A | 225 | 28.253 | 44.658 | 27.177 | 1.00 | 30.23 | N |
| ATOM | 1699 | CA  | GLU | A | 225 | 27.873 | 45.951 | 27.753 | 1.00 | 31.35 | C |
| ATOM | 1700 | C   | GLU | A | 225 | 26.362 | 46.120 | 27.909 | 1.00 | 30.48 | C |
| ATOM | 1701 | O   | GLU | A | 225 | 25.925 | 46.920 | 28.738 | 1.00 | 28.49 | O |
| ATOM | 1702 | CB  | GLU | A | 225 | 28.401 | 47.130 | 26.927 | 1.00 | 32.35 | C |
| ATOM | 1703 | CG  | GLU | A | 225 | 29.894 | 47.356 | 27.083 | 1.00 | 37.72 | C |
| ATOM | 1704 | CD  | GLU | A | 225 | 30.327 | 48.801 | 27.406 | 1.00 | 45.22 | C |
| ATOM | 1705 | OE1 | GLU | A | 225 | 29.848 | 49.472 | 28.389 | 1.00 | 44.87 | O |
| ATOM | 1706 | OE2 | GLU | A | 225 | 31.230 | 49.248 | 26.665 | 1.00 | 54.04 | O |
| ATOM | 1707 | N   | CYS | A | 226 | 25.579 | 45.375 | 27.116 | 1.00 | 29.44 | N |
| ATOM | 1708 | CA  | CYS | A | 226 | 24.132 | 45.532 | 27.155 | 1.00 | 28.60 | C |
| ATOM | 1709 | C   | CYS | A | 226 | 23.429 | 44.524 | 28.056 | 1.00 | 28.86 | C |
| ATOM | 1710 | O   | CYS | A | 226 | 22.236 | 44.716 | 28.352 | 1.00 | 27.16 | O |
| ATOM | 1711 | CB  | CYS | A | 226 | 23.541 | 45.373 | 25.767 | 1.00 | 29.07 | C |
| ATOM | 1712 | SG  | CYS | A | 226 | 24.193 | 46.391 | 24.441 | 1.00 | 29.66 | S |
| ATOM | 1713 | N   | LEU | A | 227 | 24.133 | 43.455 | 28.483 | 1.00 | 28.37 | N |
| ATOM | 1714 | CA  | LEU | A | 227 | 23.469 | 42.390 | 29.242 | 1.00 | 28.53 | C |
| ATOM | 1715 | C   | LEU | A | 227 | 23.760 | 42.287 | 30.737 | 1.00 | 27.80 | C |
| ATOM | 1716 | O   | LEU | A | 227 | 23.117 | 41.540 | 31.465 | 1.00 | 26.98 | O |
| ATOM | 1717 | CB  | LEU | A | 227 | 23.701 | 41.062 | 28.531 | 1.00 | 28.86 | C |
| ATOM | 1718 | CG  | LEU | A | 227 | 22.853 | 41.135 | 27.246 | 1.00 | 30.66 | C |
| ATOM | 1719 | CD1 | LEU | A | 227 | 23.335 | 40.152 | 26.186 | 1.00 | 32.05 | C |
| ATOM | 1720 | CD2 | LEU | A | 227 | 21.389 | 40.812 | 27.590 | 1.00 | 30.73 | C |
| ATOM | 1721 | N   | TYR | A | 228 | 24.760 | 43.016 | 31.170 | 1.00 | 28.05 | N |
| ATOM | 1722 | CA  | TYR | A | 228 | 25.034 | 43.219 | 32.596 | 1.00 | 28.59 | C |
| ATOM | 1723 | C   | TYR | A | 228 | 25.051 | 41.978 | 33.504 | 1.00 | 29.27 | C |
| ATOM | 1724 | O   | TYR | A | 228 | 24.253 | 41.863 | 34.483 | 1.00 | 29.59 | O |
| ATOM | 1725 | CB  | TYR | A | 228 | 24.026 | 44.213 | 33.157 | 1.00 | 28.04 | C |
| ATOM | 1726 | CG  | TYR | A | 228 | 24.019 | 45.556 | 32.464 | 1.00 | 28.00 | C |
| ATOM | 1727 | CD1 | TYR | A | 228 | 24.839 | 46.584 | 32.881 | 1.00 | 27.54 | C |
| ATOM | 1728 | CD2 | TYR | A | 228 | 23.177 | 45.799 | 31.389 | 1.00 | 28.83 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1729 | CE1 | TYR | A | 228 | 24.826 | 47.828 | 32.248 | 1.00 | 27.44 | C |
| ATOM | 1730 | CE2 | TYR | A | 228 | 23.160 | 47.018 | 30.745 | 1.00 | 27.63 | C |
| ATOM | 1731 | CZ  | TYR | A | 228 | 23.964 | 48.040 | 31.186 | 1.00 | 29.01 | C |
| ATOM | 1732 | OH  | TYR | A | 228 | 23.924 | 49.260 | 30.536 | 1.00 | 28.98 | O |
| ATOM | 1733 | N   | PRO | A | 229 | 26.009 | 41.101 | 33.261 | 1.00 | 28.11 | N |
| ATOM | 1734 | CA  | PRO | A | 229 | 26.146 | 39.900 | 34.082 | 1.00 | 28.54 | C |
| ATOM | 1735 | C   | PRO | A | 229 | 26.424 | 40.223 | 35.534 | 1.00 | 27.88 | C |
| ATOM | 1736 | O   | PRO | A | 229 | 27.085 | 41.212 | 35.786 | 1.00 | 28.01 | O |
| ATOM | 1737 | CB  | PRO | A | 229 | 27.396 | 39.214 | 33.494 | 1.00 | 28.67 | C |
| ATOM | 1738 | CG  | PRO | A | 229 | 28.116 | 40.314 | 32.802 | 1.00 | 28.96 | C |
| ATOM | 1739 | CD  | PRO | A | 229 | 27.046 | 41.191 | 32.231 | 1.00 | 28.25 | C |
| ATOM | 1740 | N   | TYR | A | 230 | 25.981 | 39.372 | 36.453 | 1.00 | 26.80 | N |
| ATOM | 1741 | CA  | TYR | A | 230 | 26.296 | 39.542 | 37.840 | 1.00 | 25.91 | C |
| ATOM | 1742 | C   | TYR | A | 230 | 27.838 | 39.508 | 38.028 | 1.00 | 25.72 | C |
| ATOM | 1743 | O   | TYR | A | 230 | 28.582 | 39.094 | 37.167 | 1.00 | 25.79 | O |
| ATOM | 1744 | CB  | TYR | A | 230 | 25.673 | 38.431 | 38.677 | 1.00 | 25.13 | C |
| ATOM | 1745 | CG  | TYR | A | 230 | 24.193 | 38.523 | 38.900 | 1.00 | 24.95 | C |
| ATOM | 1746 | CD1 | TYR | A | 230 | 23.289 | 38.036 | 37.933 | 1.00 | 24.25 | C |
| ATOM | 1747 | CD2 | TYR | A | 230 | 23.675 | 39.063 | 40.090 | 1.00 | 25.16 | C |
| ATOM | 1748 | CE1 | TYR | A | 230 | 21.944 | 38.105 | 38.139 | 1.00 | 24.40 | C |
| ATOM | 1749 | CE2 | TYR | A | 230 | 22.311 | 39.114 | 40.320 | 1.00 | 23.86 | C |
| ATOM | 1750 | CZ  | TYR | A | 230 | 21.464 | 38.647 | 39.336 | 1.00 | 26.74 | C |
| ATOM | 1751 | OH  | TYR | A | 230 | 20.122 | 38.713 | 39.501 | 1.00 | 34.04 | O |
| ATOM | 1752 | N   | PRO | A | 231 | 28.309 | 39.966 | 39.167 | 1.00 | 25.05 | N |
| ATOM | 1753 | CA  | PRO | A | 231 | 29.711 | 39.806 | 39.517 | 1.00 | 24.73 | C |
| ATOM | 1754 | C   | PRO | A | 231 | 30.151 | 38.318 | 39.500 | 1.00 | 24.94 | C |
| ATOM | 1755 | O   | PRO | A | 231 | 29.359 | 37.410 | 39.817 | 1.00 | 24.30 | O |
| ATOM | 1756 | CB  | PRO | A | 231 | 29.760 | 40.353 | 40.957 | 1.00 | 25.28 | C |
| ATOM | 1757 | CG  | PRO | A | 231 | 28.613 | 41.331 | 41.016 | 1.00 | 25.28 | C |
| ATOM | 1758 | CD  | PRO | A | 231 | 27.535 | 40.687 | 40.198 | 1.00 | 24.73 | C |
| ATOM | 1759 | N   | VAL | A | 232 | 31.419 | 38.086 | 39.173 | 1.00 | 23.75 | N |
| ATOM | 1760 | CA  | VAL | A | 232 | 31.898 | 36.766 | 39.055 | 1.00 | 24.45 | C |
| ATOM | 1761 | C   | VAL | A | 232 | 31.725 | 35.935 | 40.351 | 1.00 | 24.83 | C |
| ATOM | 1762 | O   | VAL | A | 232 | 31.402 | 34.754 | 40.263 | 1.00 | 24.83 | O |
| ATOM | 1763 | CB  | VAL | A | 232 | 33.375 | 36.761 | 38.582 | 1.00 | 25.13 | C |
| ATOM | 1764 | CG1 | VAL | A | 232 | 33.974 | 35.405 | 38.828 | 1.00 | 23.91 | C |
| ATOM | 1765 | CG2 | VAL | A | 232 | 33.481 | 37.091 | 37.092 | 1.00 | 23.86 | C |
| ATOM | 1766 | N   | HIS | A | 233 | 31.886 | 36.540 | 41.525 | 1.00 | 25.24 | N |
| ATOM | 1767 | CA  | HIS | A | 233 | 31.766 | 35.806 | 42.790 | 1.00 | 26.43 | C |
| ATOM | 1768 | C   | HIS | A | 233 | 30.321 | 35.656 | 43.304 | 1.00 | 26.47 | C |
| ATOM | 1769 | O   | HIS | A | 233 | 30.052 | 34.986 | 44.289 | 1.00 | 26.08 | O |
| ATOM | 1770 | CB  | HIS | A | 233 | 32.617 | 36.475 | 43.855 | 1.00 | 26.65 | C |
| ATOM | 1771 | CG  | HIS | A | 233 | 34.078 | 36.428 | 43.564 | 1.00 | 28.51 | C |
| ATOM | 1772 | ND1 | HIS | A | 233 | 34.764 | 37.493 | 43.013 | 1.00 | 30.95 | N |
| ATOM | 1773 | CD2 | HIS | A | 233 | 34.987 | 35.435 | 43.730 | 1.00 | 29.75 | C |
| ATOM | 1774 | CE1 | HIS | A | 233 | 36.043 | 37.169 | 42.888 | 1.00 | 31.18 | C |
| ATOM | 1775 | NE2 | HIS | A | 233 | 36.201 | 35.919 | 43.302 | 1.00 | 32.10 | N |
| ATOM | 1776 | N   | HIS | A | 234 | 29.391 | 36.283 | 42.626 | 1.00 | 26.94 | N |
| ATOM | 1777 | CA  | HIS | A | 234 | 27.999 | 36.141 | 42.983 | 1.00 | 27.89 | C |
| ATOM | 1778 | C   | HIS | A | 234 | 27.456 | 34.838 | 42.411 | 1.00 | 27.85 | C |
| ATOM | 1779 | O   | HIS | A | 234 | 27.871 | 34.403 | 41.384 | 1.00 | 27.14 | O |
| ATOM | 1780 | CB  | HIS | A | 234 | 27.219 | 37.258 | 42.372 | 1.00 | 28.20 | C |
| ATOM | 1781 | CG  | HIS | A | 234 | 25.782 | 37.279 | 42.748 | 1.00 | 27.95 | C |
| ATOM | 1782 | ND1 | HIS | A | 234 | 24.840 | 36.514 | 42.092 | 1.00 | 30.05 | N |
| ATOM | 1783 | CD2 | HIS | A | 234 | 25.105 | 38.057 | 43.624 | 1.00 | 26.43 | C |
| ATOM | 1784 | CE1 | HIS | A | 234 | 23.644 | 36.789 | 42.588 | 1.00 | 29.87 | C |
| ATOM | 1785 | NE2 | HIS | A | 234 | 23.781 | 37.714 | 43.524 | 1.00 | 27.85 | N |
| ATOM | 1786 | N   | PRO | A | 235 | 26.561 | 34.197 | 43.130 | 1.00 | 28.44 | N |
| ATOM | 1787 | CA  | PRO | A | 235 | 26.018 | 32.929 | 42.678 | 1.00 | 28.87 | C |
| ATOM | 1788 | C   | PRO | A | 235 | 25.431 | 32.956 | 41.294 | 1.00 | 28.34 | C |
| ATOM | 1789 | O   | PRO | A | 235 | 25.387 | 31.884 | 40.716 | 1.00 | 28.04 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1790 | CB  | PRO | A | 235 | 24.931 | 32.636 | 43.713 | 1.00 | 29.59 | C |
| ATOM | 1791 | CG  | PRO | A | 235 | 25.473 | 33.290 | 44.975 | 1.00 | 29.10 | C |
| ATOM | 1792 | CD  | PRO | A | 235 | 26.059 | 34.571 | 44.466 | 1.00 | 28.17 | C |
| ATOM | 1793 | N   | CYS | A | 236 | 25.021 | 34.112 | 40.770 | 1.00 | 27.29 | N |
| ATOM | 1794 | CA  | CYS | A | 236 | 24.447 | 34.135 | 39.455 | 1.00 | 26.15 | C |
| ATOM | 1795 | C   | CYS | A | 236 | 25.478 | 34.602 | 38.451 | 1.00 | 25.39 | C |
| ATOM | 1796 | O   | CYS | A | 236 | 25.140 | 35.102 | 37.361 | 1.00 | 26.21 | O |
| ATOM | 1797 | CB  | CYS | A | 236 | 23.158 | 34.923 | 39.436 | 1.00 | 26.36 | C |
| ATOM | 1798 | SG  | CYS | A | 236 | 21.908 | 34.207 | 40.555 | 1.00 | 29.77 | S |
| ATOM | 1799 | N   | ASP | A | 237 | 26.746 | 34.411 | 38.803 | 1.00 | 24.07 | N |
| ATOM | 1800 | CA  | ASP | A | 237 | 27.830 | 34.528 | 37.855 | 1.00 | 24.53 | C |
| ATOM | 1801 | C   | ASP | A | 237 | 27.441 | 33.977 | 36.467 | 1.00 | 24.31 | C |
| ATOM | 1802 | O   | ASP | A | 237 | 26.966 | 32.865 | 36.344 | 1.00 | 23.00 | O |
| ATOM | 1803 | CB  | ASP | A | 237 | 29.018 | 33.769 | 38.353 | 1.00 | 24.42 | C |
| ATOM | 1804 | CG  | ASP | A | 237 | 30.233 | 33.850 | 37.414 | 1.00 | 28.30 | C |
| ATOM | 1805 | OD1 | ASP | A | 237 | 30.433 | 34.877 | 36.673 | 1.00 | 29.51 | O |
| ATOM | 1806 | OD2 | ASP | A | 237 | 31.071 | 32.900 | 37.386 | 1.00 | 29.51 | O |
| ATOM | 1807 | N   | ARG | A | 238 | 27.633 | 34.803 | 35.445 | 1.00 | 24.85 | N |
| ATOM | 1808 | CA  | ARG | A | 238 | 27.388 | 34.434 | 34.041 | 1.00 | 26.59 | C |
| ATOM | 1809 | C   | ARG | A | 238 | 25.921 | 34.663 | 33.595 | 1.00 | 25.95 | C |
| ATOM | 1810 | O   | ARG | A | 238 | 25.647 | 34.628 | 32.426 | 1.00 | 26.55 | O |
| ATOM | 1811 | CB  | ARG | A | 238 | 27.834 | 32.994 | 33.737 | 1.00 | 26.57 | C |
| ATOM | 1812 | CG  | ARG | A | 238 | 29.311 | 32.758 | 33.891 | 1.00 | 27.77 | C |
| ATOM | 1813 | CD  | ARG | A | 238 | 29.727 | 31.360 | 33.399 | 1.00 | 28.78 | C |
| ATOM | 1814 | NE  | ARG | A | 238 | 29.142 | 30.434 | 34.337 | 1.00 | 33.68 | N |
| ATOM | 1815 | CZ  | ARG | A | 238 | 28.046 | 29.736 | 34.140 | 1.00 | 36.98 | C |
| ATOM | 1816 | NH1 | ARG | A | 238 | 27.383 | 29.782 | 32.980 | 1.00 | 38.06 | N |
| ATOM | 1817 | NH2 | ARG | A | 238 | 27.609 | 28.987 | 35.129 | 1.00 | 37.87 | N |
| ATOM | 1818 | N   | GLN | A | 239 | 25.012 | 34.933 | 34.516 | 1.00 | 25.97 | N |
| ATOM | 1819 | CA  | GLN | A | 239 | 23.634 | 35.245 | 34.152 | 1.00 | 26.05 | C |
| ATOM | 1820 | C   | GLN | A | 239 | 23.478 | 36.776 | 34.037 | 1.00 | 26.67 | C |
| ATOM | 1821 | O   | GLN | A | 239 | 24.196 | 37.531 | 34.699 | 1.00 | 27.33 | O |
| ATOM | 1822 | CB  | GLN | A | 239 | 22.663 | 34.724 | 35.201 | 1.00 | 25.55 | C |
| ATOM | 1823 | CG  | GLN | A | 239 | 23.027 | 33.417 | 35.843 | 1.00 | 27.73 | C |
| ATOM | 1824 | CD  | GLN | A | 239 | 23.246 | 32.282 | 34.859 | 1.00 | 31.42 | C |
| ATOM | 1825 | OE1 | GLN | A | 239 | 22.332 | 31.881 | 34.133 | 1.00 | 34.43 | O |
| ATOM | 1826 | NE2 | GLN | A | 239 | 24.457 | 31.761 | 34.835 | 1.00 | 31.35 | N |
| ATOM | 1827 | N   | SER | A | 240 | 22.569 | 37.233 | 33.185 | 1.00 | 26.94 | N |
| ATOM | 1828 | CA  | SER | A | 240 | 22.293 | 38.653 | 33.034 | 1.00 | 26.93 | C |
| ATOM | 1829 | C   | SER | A | 240 | 21.490 | 39.118 | 34.229 | 1.00 | 26.78 | C |
| ATOM | 1830 | O   | SER | A | 240 | 20.642 | 38.389 | 34.703 | 1.00 | 27.00 | O |
| ATOM | 1831 | CB  | SER | A | 240 | 21.414 | 38.891 | 31.818 | 1.00 | 26.95 | C |
| ATOM | 1832 | OG  | SER | A | 240 | 20.916 | 40.234 | 31.804 | 1.00 | 27.75 | O |
| ATOM | 1833 | N   | GLN | A | 241 | 21.733 | 40.331 | 34.696 | 1.00 | 26.90 | N |
| ATOM | 1834 | CA  | GLN | A | 241 | 20.963 | 40.903 | 35.816 | 1.00 | 27.25 | C |
| ATOM | 1835 | C   | GLN | A | 241 | 19.632 | 41.520 | 35.311 | 1.00 | 27.84 | C |
| ATOM | 1836 | O   | GLN | A | 241 | 18.763 | 41.866 | 36.104 | 1.00 | 27.28 | O |
| ATOM | 1837 | CB  | GLN | A | 241 | 21.734 | 42.009 | 36.546 | 1.00 | 26.21 | C |
| ATOM | 1838 | CG  | GLN | A | 241 | 22.971 | 41.636 | 37.344 | 1.00 | 26.53 | C |
| ATOM | 1839 | CD  | GLN | A | 241 | 23.740 | 42.877 | 37.817 | 1.00 | 26.65 | C |
| ATOM | 1840 | OE1 | GLN | A | 241 | 23.436 | 43.425 | 38.859 | 1.00 | 31.02 | O |
| ATOM | 1841 | NE2 | GLN | A | 241 | 24.714 | 43.318 | 37.048 | 1.00 | 28.00 | N |
| ATOM | 1842 | N   | VAL | A | 242 | 19.464 | 41.657 | 34.004 | 1.00 | 28.19 | N |
| ATOM | 1843 | CA  | VAL | A | 242 | 18.284 | 42.335 | 33.552 | 1.00 | 28.55 | C |
| ATOM | 1844 | C   | VAL | A | 242 | 17.117 | 41.409 | 33.563 | 1.00 | 28.88 | C |
| ATOM | 1845 | O   | VAL | A | 242 | 17.198 | 40.314 | 33.053 | 1.00 | 28.92 | O |
| ATOM | 1846 | CB  | VAL | A | 242 | 18.422 | 42.770 | 32.093 | 1.00 | 29.31 | C |
| ATOM | 1847 | CG1 | VAL | A | 242 | 17.165 | 43.549 | 31.647 | 1.00 | 27.90 | C |
| ATOM | 1848 | CG2 | VAL | A | 242 | 19.711 | 43.530 | 31.866 | 1.00 | 28.67 | C |
| ATOM | 1849 | N   | ASP | A | 243 | 16.009 | 41.862 | 34.113 | 1.00 | 28.55 | N |
| ATOM | 1850 | CA  | ASP | A | 243 | 14.766 | 41.103 | 34.052 | 1.00 | 27.62 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1851 | C   | ASP | A | 243 | 14.121 | 41.396 | 32.709 | 1.00 | 27.45 | C |
| ATOM | 1852 | O   | ASP | A | 243 | 13.579 | 42.480 | 32.452 | 1.00 | 25.90 | O |
| ATOM | 1853 | CB  | ASP | A | 243 | 13.876 | 41.560 | 35.193 | 1.00 | 27.99 | C |
| ATOM | 1854 | CG  | ASP | A | 243 | 12.509 | 40.945 | 35.177 | 1.00 | 29.40 | C |
| ATOM | 1855 | OD1 | ASP | A | 243 | 12.096 | 40.291 | 34.179 | 1.00 | 31.46 | O |
| ATOM | 1856 | OD2 | ASP | A | 243 | 11.747 | 41.110 | 36.161 | 1.00 | 32.65 | O |
| ATOM | 1857 | N   | PHE | A | 244 | 14.180 | 40.419 | 31.825 | 1.00 | 28.27 | N |
| ATOM | 1858 | CA  | PHE | A | 244 | 13.656 | 40.603 | 30.496 | 1.00 | 28.92 | C |
| ATOM | 1859 | C   | PHE | A | 244 | 12.172 | 40.975 | 30.481 | 1.00 | 30.32 | C |
| ATOM | 1860 | O   | PHE | A | 244 | 11.728 | 41.643 | 29.561 | 1.00 | 31.01 | O |
| ATOM | 1861 | CB  | PHE | A | 244 | 13.900 | 39.369 | 29.657 | 1.00 | 29.32 | C |
| ATOM | 1862 | CG  | PHE | A | 244 | 15.255 | 39.298 | 29.053 | 1.00 | 28.51 | C |
| ATOM | 1863 | CD1 | PHE | A | 244 | 16.397 | 39.628 | 29.775 | 1.00 | 31.29 | C |
| ATOM | 1864 | CD2 | PHE | A | 244 | 15.399 | 38.853 | 27.793 | 1.00 | 28.23 | C |
| ATOM | 1865 | CE1 | PHE | A | 244 | 17.649 | 39.535 | 29.196 | 1.00 | 29.39 | C |
| ATOM | 1866 | CE2 | PHE | A | 244 | 16.654 | 38.736 | 27.229 | 1.00 | 30.79 | C |
| ATOM | 1867 | CZ  | PHE | A | 244 | 17.759 | 39.107 | 27.919 | 1.00 | 29.44 | C |
| ATOM | 1868 | N   | ASP | A | 245 | 11.401 | 40.551 | 31.482 | 1.00 | 31.22 | N |
| ATOM | 1869 | CA  | ASP | A | 245 | 10.007 | 40.913 | 31.544 | 1.00 | 31.40 | C |
| ATOM | 1870 | C   | ASP | A | 245 | 9.770  | 42.349 | 32.032 | 1.00 | 31.91 | C |
| ATOM | 1871 | O   | ASP | A | 245 | 8.704  | 42.891 | 31.786 | 1.00 | 30.40 | O |
| ATOM | 1872 | CB  | ASP | A | 245 | 9.263  | 39.968 | 32.467 | 1.00 | 32.57 | C |
| ATOM | 1873 | CG  | ASP | A | 245 | 9.292  | 38.546 | 31.988 | 1.00 | 33.29 | C |
| ATOM | 1874 | OD1 | ASP | A | 245 | 9.289  | 38.333 | 30.768 | 1.00 | 35.51 | O |
| ATOM | 1875 | OD2 | ASP | A | 245 | 9.348  | 37.577 | 32.764 | 1.00 | 35.50 | O |
| ATOM | 1876 | N   | ASN | A | 246 | 10.735 | 42.954 | 32.731 | 1.00 | 32.07 | N |
| ATOM | 1877 | CA  | ASN | A | 246 | 10.562 | 44.310 | 33.244 | 1.00 | 33.10 | C |
| ATOM | 1878 | C   | ASN | A | 246 | 11.884 | 45.016 | 33.384 | 1.00 | 32.49 | C |
| ATOM | 1879 | O   | ASN | A | 246 | 12.400 | 45.179 | 34.476 | 1.00 | 33.20 | O |
| ATOM | 1880 | CB  | ASN | A | 246 | 9.873  | 44.296 | 34.603 | 1.00 | 33.31 | C |
| ATOM | 1881 | CG  | ASN | A | 246 | 9.555  | 45.716 | 35.110 | 1.00 | 39.27 | C |
| ATOM | 1882 | OD1 | ASN | A | 246 | 9.331  | 46.678 | 34.313 | 1.00 | 43.28 | O |
| ATOM | 1883 | ND2 | ASN | A | 246 | 9.551  | 45.867 | 36.445 | 1.00 | 44.32 | N |
| ATOM | 1884 | N   | PRO | A | 247 | 12.472 | 45.374 | 32.265 | 1.00 | 31.66 | N |
| ATOM | 1885 | CA  | PRO | A | 247 | 13.822 | 45.936 | 32.263 | 1.00 | 31.26 | C |
| ATOM | 1886 | C   | PRO | A | 247 | 13.924 | 47.298 | 32.933 | 1.00 | 31.58 | C |
| ATOM | 1887 | O   | PRO | A | 247 | 13.185 | 48.211 | 32.629 | 1.00 | 31.85 | O |
| ATOM | 1888 | CB  | PRO | A | 247 | 14.161 | 46.082 | 30.782 | 1.00 | 31.22 | C |
| ATOM | 1889 | CG  | PRO | A | 247 | 13.017 | 45.510 | 30.022 | 1.00 | 31.05 | C |
| ATOM | 1890 | CD  | PRO | A | 247 | 11.894 | 45.216 | 30.928 | 1.00 | 31.01 | C |
| ATOM | 1891 | N   | ASP | A | 248 | 14.893 | 47.422 | 33.815 | 1.00 | 31.35 | N |
| ATOM | 1892 | CA  | ASP | A | 248 | 15.161 | 48.643 | 34.467 | 1.00 | 31.48 | C |
| ATOM | 1893 | C   | ASP | A | 248 | 16.222 | 49.413 | 33.650 | 1.00 | 31.23 | C |
| ATOM | 1894 | O   | ASP | A | 248 | 17.422 | 49.217 | 33.784 | 1.00 | 30.76 | O |
| ATOM | 1895 | CB  | ASP | A | 248 | 15.646 | 48.310 | 35.850 | 1.00 | 31.60 | C |
| ATOM | 1896 | CG  | ASP | A | 248 | 15.745 | 49.504 | 36.720 | 1.00 | 33.62 | C |
| ATOM | 1897 | OD1 | ASP | A | 248 | 16.020 | 50.619 | 36.201 | 1.00 | 34.39 | O |
| ATOM | 1898 | OD2 | ASP | A | 248 | 15.578 | 49.395 | 37.949 | 1.00 | 38.39 | O |
| ATOM | 1899 | N   | TYR | A | 249 | 15.764 | 50.285 | 32.783 | 1.00 | 31.95 | N |
| ATOM | 1900 | CA  | TYR | A | 249 | 16.676 | 51.053 | 31.942 | 1.00 | 32.80 | C |
| ATOM | 1901 | C   | TYR | A | 249 | 17.534 | 52.052 | 32.714 | 1.00 | 33.92 | C |
| ATOM | 1902 | O   | TYR | A | 249 | 18.558 | 52.490 | 32.203 | 1.00 | 34.33 | O |
| ATOM | 1903 | CB  | TYR | A | 249 | 15.906 | 51.732 | 30.825 | 1.00 | 32.56 | C |
| ATOM | 1904 | CG  | TYR | A | 249 | 15.183 | 50.751 | 29.928 | 1.00 | 31.41 | C |
| ATOM | 1905 | CD1 | TYR | A | 249 | 15.859 | 49.695 | 29.316 | 1.00 | 30.27 | C |
| ATOM | 1906 | CD2 | TYR | A | 249 | 13.845 | 50.868 | 29.704 | 1.00 | 29.24 | C |
| ATOM | 1907 | CE1 | TYR | A | 249 | 15.205 | 48.814 | 28.478 | 1.00 | 29.30 | C |
| ATOM | 1908 | CE2 | TYR | A | 249 | 13.178 | 49.968 | 28.894 | 1.00 | 29.24 | C |
| ATOM | 1909 | CZ  | TYR | A | 249 | 13.858 | 48.947 | 28.285 | 1.00 | 29.20 | C |
| ATOM | 1910 | OH  | TYR | A | 249 | 13.173 | 48.078 | 27.452 | 1.00 | 29.69 | O |
| ATOM | 1911 | N   | GLU | A | 250 | 17.155 | 52.369 | 33.952 | 1.00 | 34.69 | N |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1912 | CA  | GLU | A | 250 | 17.994 | 53.202 | 34.789 | 1.00 | 35.66 | C |
| ATOM | 1913 | C   | GLU | A | 250 | 19.249 | 52.494 | 35.235 | 1.00 | 34.69 | C |
| ATOM | 1914 | O   | GLU | A | 250 | 20.313 | 53.077 | 35.207 | 1.00 | 34.29 | O |
| ATOM | 1915 | CB  | GLU | A | 250 | 17.252 | 53.685 | 36.021 | 1.00 | 36.82 | C |
| ATOM | 1916 | CG  | GLU | A | 250 | 16.115 | 54.609 | 35.650 | 1.00 | 41.99 | C |
| ATOM | 1917 | CD  | GLU | A | 250 | 15.554 | 55.360 | 36.827 | 1.00 | 48.02 | C |
| ATOM | 1918 | OE1 | GLU | A | 250 | 16.114 | 55.275 | 37.949 | 1.00 | 53.95 | O |
| ATOM | 1919 | OE2 | GLU | A | 250 | 14.543 | 56.043 | 36.614 | 1.00 | 52.47 | O |
| ATOM | 1920 | N   | ARG | A | 251 | 19.139 | 51.254 | 35.691 | 1.00 | 33.87 | N |
| ATOM | 1921 | CA  | ARG | A | 251 | 20.335 | 50.550 | 36.088 | 1.00 | 33.26 | C |
| ATOM | 1922 | C   | ARG | A | 251 | 21.013 | 49.992 | 34.873 | 1.00 | 32.36 | C |
| ATOM | 1923 | O   | ARG | A | 251 | 22.210 | 49.914 | 34.849 | 1.00 | 32.79 | O |
| ATOM | 1924 | CB  | ARG | A | 251 | 20.040 | 49.425 | 37.066 | 1.00 | 34.36 | C |
| ATOM | 1925 | CG  | ARG | A | 251 | 19.476 | 49.895 | 38.425 | 1.00 | 36.13 | C |
| ATOM | 1926 | CD  | ARG | A | 251 | 18.966 | 48.771 | 39.339 | 1.00 | 39.31 | C |
| ATOM | 1927 | NE  | ARG | A | 251 | 20.052 | 47.860 | 39.733 | 1.00 | 42.09 | N |
| ATOM | 1928 | CZ  | ARG | A | 251 | 19.890 | 46.563 | 39.964 | 1.00 | 41.90 | C |
| ATOM | 1929 | NH1 | ARG | A | 251 | 18.696 | 46.006 | 39.843 | 1.00 | 41.62 | N |
| ATOM | 1930 | NH2 | ARG | A | 251 | 20.932 | 45.815 | 40.296 | 1.00 | 41.98 | N |
| ATOM | 1931 | N   | PHE | A | 252 | 20.272 | 49.654 | 33.825 | 1.00 | 31.66 | N |
| ATOM | 1932 | CA  | PHE | A | 252 | 20.879 | 48.977 | 32.677 | 1.00 | 30.28 | C |
| ATOM | 1933 | C   | PHE | A | 252 | 20.528 | 49.651 | 31.347 | 1.00 | 29.72 | C |
| ATOM | 1934 | O   | PHE | A | 252 | 19.882 | 49.096 | 30.483 | 1.00 | 29.84 | O |
| ATOM | 1935 | CB  | PHE | A | 252 | 20.420 | 47.531 | 32.675 | 1.00 | 29.99 | C |
| ATOM | 1936 | CG  | PHE | A | 252 | 20.405 | 46.864 | 34.050 | 1.00 | 29.63 | C |
| ATOM | 1937 | CD1 | PHE | A | 252 | 21.562 | 46.717 | 34.796 | 1.00 | 29.74 | C |
| ATOM | 1938 | CD2 | PHE | A | 252 | 19.238 | 46.317 | 34.554 | 1.00 | 31.30 | C |
| ATOM | 1939 | CE1 | PHE | A | 252 | 21.546 | 46.067 | 36.039 | 1.00 | 30.44 | C |
| ATOM | 1940 | CE2 | PHE | A | 252 | 19.199 | 45.668 | 35.805 | 1.00 | 31.42 | C |
| ATOM | 1941 | CZ  | PHE | A | 252 | 20.356 | 45.551 | 36.550 | 1.00 | 32.04 | C |
| ATOM | 1942 | N   | PRO | A | 253 | 21.034 | 50.844 | 31.155 | 1.00 | 29.72 | N |
| ATOM | 1943 | CA  | PRO | A | 253 | 20.607 | 51.662 | 30.022 | 1.00 | 28.89 | C |
| ATOM | 1944 | C   | PRO | A | 253 | 20.953 | 50.996 | 28.689 | 1.00 | 29.46 | C |
| ATOM | 1945 | O   | PRO | A | 253 | 20.166 | 51.061 | 27.722 | 1.00 | 28.81 | O |
| ATOM | 1946 | CB  | PRO | A | 253 | 21.361 | 52.975 | 30.240 | 1.00 | 28.37 | C |
| ATOM | 1947 | CG  | PRO | A | 253 | 22.543 | 52.614 | 31.155 | 1.00 | 27.97 | C |
| ATOM | 1948 | CD  | PRO | A | 253 | 22.136 | 51.463 | 31.942 | 1.00 | 29.24 | C |
| ATOM | 1949 | N   | ASN | A | 254 | 22.093 | 50.323 | 28.590 | 1.00 | 29.37 | N |
| ATOM | 1950 | CA  | ASN | A | 254 | 22.401 | 49.742 | 27.274 | 1.00 | 28.85 | C |
| ATOM | 1951 | C   | ASN | A | 254 | 21.547 | 48.529 | 26.902 | 1.00 | 28.28 | C |
| ATOM | 1952 | O   | ASN | A | 254 | 21.663 | 47.970 | 25.794 | 1.00 | 27.47 | O |
| ATOM | 1953 | CB  | ASN | A | 254 | 23.874 | 49.407 | 27.122 | 1.00 | 28.84 | C |
| ATOM | 1954 | CG  | ASN | A | 254 | 24.745 | 50.654 | 26.996 | 1.00 | 29.96 | C |
| ATOM | 1955 | OD1 | ASN | A | 254 | 25.622 | 50.882 | 27.834 | 1.00 | 31.21 | O |
| ATOM | 1956 | ND2 | ASN | A | 254 | 24.531 | 51.443 | 25.931 | 1.00 | 29.17 | N |
| ATOM | 1957 | N   | PHE | A | 255 | 20.687 | 48.091 | 27.797 | 1.00 | 27.30 | N |
| ATOM | 1958 | CA  | PHE | A | 255 | 19.801 | 47.006 | 27.368 | 1.00 | 27.53 | C |
| ATOM | 1959 | C   | PHE | A | 255 | 18.844 | 47.512 | 26.283 | 1.00 | 26.80 | C |
| ATOM | 1960 | O   | PHE | A | 255 | 18.193 | 46.750 | 25.603 | 1.00 | 27.22 | O |
| ATOM | 1961 | CB  | PHE | A | 255 | 19.015 | 46.448 | 28.538 | 1.00 | 27.48 | C |
| ATOM | 1962 | CG  | PHE | A | 255 | 18.282 | 45.250 | 28.198 | 1.00 | 26.63 | C |
| ATOM | 1963 | CD1 | PHE | A | 255 | 18.950 | 44.073 | 27.998 | 1.00 | 29.74 | C |
| ATOM | 1964 | CD2 | PHE | A | 255 | 16.935 | 45.288 | 28.039 | 1.00 | 26.29 | C |
| ATOM | 1965 | CE1 | PHE | A | 255 | 18.273 | 42.947 | 27.681 | 1.00 | 29.50 | C |
| ATOM | 1966 | CE2 | PHE | A | 255 | 16.261 | 44.192 | 27.692 | 1.00 | 26.21 | C |
| ATOM | 1967 | CZ  | PHE | A | 255 | 16.917 | 43.012 | 27.518 | 1.00 | 30.10 | C |
| ATOM | 1968 | N   | GLN | A | 256 | 18.776 | 48.818 | 26.125 | 1.00 | 26.57 | N |
| ATOM | 1969 | CA  | GLN | A | 256 | 17.918 | 49.429 | 25.137 | 1.00 | 26.55 | C |
| ATOM | 1970 | C   | GLN | A | 256 | 18.522 | 49.253 | 23.745 | 1.00 | 26.46 | C |
| ATOM | 1971 | O   | GLN | A | 256 | 17.881 | 49.560 | 22.771 | 1.00 | 24.39 | O |
| ATOM | 1972 | CB  | GLN | A | 256 | 17.756 | 50.933 | 25.423 | 1.00 | 26.18 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1973 | CG  | GLN | A | 256 | 16.656 | 51.226 | 26.406 | 1.00 | 28.72 | C |
| ATOM | 1974 | CD  | GLN | A | 256 | 16.721 | 52.636 | 27.028 | 1.00 | 29.64 | C |
| ATOM | 1975 | OE1 | GLN | A | 256 | 15.737 | 53.358 | 27.005 | 1.00 | 32.56 | O |
| ATOM | 1976 | NE2 | GLN | A | 256 | 17.861 | 52.999 | 27.590 | 1.00 | 26.88 | N |
| ATOM | 1977 | N   | ASN | A | 257 | 19.774 | 48.809 | 23.694 | 1.00 | 27.86 | N |
| ATOM | 1978 | CA  | ASN | A | 257 | 20.509 | 48.611 | 22.452 | 1.00 | 29.22 | C |
| ATOM | 1979 | C   | ASN | A | 257 | 20.733 | 47.143 | 22.116 | 1.00 | 30.46 | C |
| ATOM | 1980 | O   | ASN | A | 257 | 21.399 | 46.855 | 21.132 | 1.00 | 32.28 | O |
| ATOM | 1981 | CB  | ASN | A | 257 | 21.897 | 49.232 | 22.510 | 1.00 | 28.50 | C |
| ATOM | 1982 | CG  | ASN | A | 257 | 21.878 | 50.666 | 22.890 | 1.00 | 29.30 | C |
| ATOM | 1983 | OD1 | ASN | A | 257 | 22.329 | 51.025 | 23.989 | 1.00 | 27.33 | O |
| ATOM | 1984 | ND2 | ASN | A | 257 | 21.382 | 51.523 | 21.982 | 1.00 | 25.68 | N |
| ATOM | 1985 | N   | VAL | A | 258 | 20.200 | 46.213 | 22.900 | 1.00 | 31.51 | N |
| ATOM | 1986 | CA  | VAL | A | 258 | 20.432 | 44.791 | 22.623 | 1.00 | 32.54 | C |
| ATOM | 1987 | C   | VAL | A | 258 | 19.674 | 44.295 | 21.386 | 1.00 | 32.39 | C |
| ATOM | 1988 | O   | VAL | A | 258 | 18.543 | 44.766 | 21.081 | 1.00 | 32.29 | O |
| ATOM | 1989 | CB  | VAL | A | 258 | 20.050 | 43.937 | 23.841 | 1.00 | 33.12 | C |
| ATOM | 1990 | CG1 | VAL | A | 258 | 18.546 | 43.818 | 23.986 | 1.00 | 32.40 | C |
| ATOM | 1991 | CG2 | VAL | A | 258 | 20.646 | 42.566 | 23.686 | 1.00 | 36.78 | C |
| ATOM | 1992 | N   | VAL | A | 259 | 20.302 | 43.386 | 20.654 | 1.00 | 32.45 | N |
| ATOM | 1993 | CA  | VAL | A | 259 | 19.682 | 42.796 | 19.448 | 1.00 | 32.96 | C |
| ATOM | 1994 | C   | VAL | A | 259 | 19.943 | 41.301 | 19.391 | 1.00 | 33.08 | C |
| ATOM | 1995 | O   | VAL | A | 259 | 21.074 | 40.878 | 19.351 | 1.00 | 33.50 | O |
| ATOM | 1996 | CB  | VAL | A | 259 | 20.269 | 43.401 | 18.172 | 1.00 | 33.19 | C |
| ATOM | 1997 | CG1 | VAL | A | 259 | 19.625 | 42.771 | 16.962 | 1.00 | 34.73 | C |
| ATOM | 1998 | CG2 | VAL | A | 259 | 20.054 | 44.901 | 18.143 | 1.00 | 32.25 | C |
| ATOM | 1999 | N   | GLY | A | 260 | 18.902 | 40.491 | 19.406 | 1.00 | 33.70 | N |
| ATOM | 2000 | CA  | GLY | A | 260 | 19.091 | 39.052 | 19.368 | 1.00 | 34.16 | C |
| ATOM | 2001 | C   | GLY | A | 260 | 19.036 | 38.327 | 18.014 | 1.00 | 33.92 | C |
| ATOM | 2002 | O   | GLY | A | 260 | 18.655 | 38.891 | 16.975 | 1.00 | 33.59 | O |
| ATOM | 2003 | N   | TYR | A | 261 | 19.469 | 37.071 | 18.052 | 1.00 | 33.14 | N |
| ATOM | 2004 | CA  | TYR | A | 261 | 19.375 | 36.157 | 16.938 | 1.00 | 33.55 | C |
| ATOM | 2005 | C   | TYR | A | 261 | 18.439 | 35.095 | 17.489 | 1.00 | 33.41 | C |
| ATOM | 2006 | O   | TYR | A | 261 | 18.700 | 34.542 | 18.561 | 1.00 | 33.67 | O |
| ATOM | 2007 | CB  | TYR | A | 261 | 20.715 | 35.508 | 16.657 | 1.00 | 33.81 | C |
| ATOM | 2008 | CG  | TYR | A | 261 | 21.758 | 36.416 | 16.061 | 1.00 | 36.80 | C |
| ATOM | 2009 | CD1 | TYR | A | 261 | 21.886 | 36.545 | 14.694 | 1.00 | 42.37 | C |
| ATOM | 2010 | CD2 | TYR | A | 261 | 22.602 | 37.139 | 16.851 | 1.00 | 38.31 | C |
| ATOM | 2011 | CE1 | TYR | A | 261 | 22.823 | 37.378 | 14.139 | 1.00 | 43.02 | C |
| ATOM | 2012 | CE2 | TYR | A | 261 | 23.556 | 37.938 | 16.312 | 1.00 | 40.85 | C |
| ATOM | 2013 | CZ  | TYR | A | 261 | 23.660 | 38.058 | 14.955 | 1.00 | 42.50 | C |
| ATOM | 2014 | OH  | TYR | A | 261 | 24.617 | 38.865 | 14.414 | 1.00 | 45.43 | O |
| ATOM | 2015 | N   | GLU | A | 262 | 17.322 | 34.832 | 16.834 | 1.00 | 32.71 | N |
| ATOM | 2016 | CA  | GLU | A | 262 | 16.394 | 33.886 | 17.438 | 1.00 | 32.21 | C |
| ATOM | 2017 | C   | GLU | A | 262 | 15.975 | 32.768 | 16.508 | 1.00 | 30.89 | C |
| ATOM | 2018 | O   | GLU | A | 262 | 16.180 | 32.819 | 15.294 | 1.00 | 30.63 | O |
| ATOM | 2019 | CB  | GLU | A | 262 | 15.196 | 34.613 | 18.049 | 1.00 | 32.16 | C |
| ATOM | 2020 | CG  | GLU | A | 262 | 13.968 | 34.753 | 17.210 | 1.00 | 30.84 | C |
| ATOM | 2021 | CD  | GLU | A | 262 | 12.818 | 35.380 | 17.992 | 1.00 | 31.21 | C |
| ATOM | 2022 | OE1 | GLU | A | 262 | 12.761 | 36.612 | 18.108 | 1.00 | 34.58 | O |
| ATOM | 2023 | OE2 | GLU | A | 262 | 11.962 | 34.663 | 18.504 | 1.00 | 29.56 | O |
| ATOM | 2024 | N   | THR | A | 263 | 15.447 | 31.746 | 17.133 | 1.00 | 28.97 | N |
| ATOM | 2025 | CA  | THR | A | 263 | 14.941 | 30.587 | 16.447 | 1.00 | 28.44 | C |
| ATOM | 2026 | C   | THR | A | 263 | 14.080 | 29.743 | 17.387 | 1.00 | 27.24 | C |
| ATOM | 2027 | O   | THR | A | 263 | 14.088 | 29.893 | 18.620 | 1.00 | 26.43 | O |
| ATOM | 2028 | CB  | THR | A | 263 | 16.093 | 29.746 | 15.902 | 1.00 | 28.50 | C |
| ATOM | 2029 | OG1 | THR | A | 263 | 15.592 | 28.798 | 14.964 | 1.00 | 27.18 | O |
| ATOM | 2030 | CG2 | THR | A | 263 | 16.697 | 28.854 | 16.975 | 1.00 | 28.63 | C |
| ATOM | 2031 | N   | VAL | A | 264 | 13.306 | 28.887 | 16.776 | 1.00 | 27.22 | N |
| ATOM | 2032 | CA  | VAL | A | 264 | 12.509 | 27.942 | 17.497 | 1.00 | 28.49 | C |
| ATOM | 2033 | C   | VAL | A | 264 | 12.925 | 26.576 | 17.022 | 1.00 | 29.10 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2034 | O   | VAL | A | 264 | 12.876 | 26.279 | 15.828 | 1.00 | 28.47 | O |
| ATOM | 2035 | CB  | VAL | A | 264 | 11.025 | 28.126 | 17.252 | 1.00 | 29.23 | C |
| ATOM | 2036 | CG1 | VAL | A | 264 | 10.259 | 26.871 | 17.767 | 1.00 | 29.07 | C |
| ATOM | 2037 | CG2 | VAL | A | 264 | 10.520 | 29.431 | 17.973 | 1.00 | 28.52 | C |
| ATOM | 2038 | N   | VAL | A | 265 | 13.401 | 25.763 | 17.954 | 1.00 | 29.56 | N |
| ATOM | 2039 | CA  | VAL | A | 265 | 13.806 | 24.413 | 17.594 | 1.00 | 29.83 | C |
| ATOM | 2040 | C   | VAL | A | 265 | 12.785 | 23.404 | 18.039 | 1.00 | 29.63 | C |
| ATOM | 2041 | O   | VAL | A | 265 | 12.188 | 23.544 | 19.105 | 1.00 | 29.93 | O |
| ATOM | 2042 | CB  | VAL | A | 265 | 15.197 | 24.015 | 18.203 | 1.00 | 29.88 | C |
| ATOM | 2043 | CG1 | VAL | A | 265 | 16.281 | 24.883 | 17.589 | 1.00 | 32.24 | C |
| ATOM | 2044 | CG2 | VAL | A | 265 | 15.234 | 24.114 | 19.712 | 1.00 | 26.80 | C |
| ATOM | 2045 | N   | GLY | A | 266 | 12.642 | 22.371 | 17.226 | 1.00 | 28.96 | N |
| ATOM | 2046 | CA  | GLY | A | 266 | 11.770 | 21.268 | 17.513 | 1.00 | 28.86 | C |
| ATOM | 2047 | C   | GLY | A | 266 | 12.463 | 19.909 | 17.428 | 1.00 | 28.32 | C |
| ATOM | 2048 | O   | GLY | A | 266 | 13.656 | 19.804 | 17.215 | 1.00 | 28.58 | O |
| ATOM | 2049 | N   | PRO | A | 267 | 11.696 | 18.852 | 17.581 | 1.00 | 28.06 | N |
| ATOM | 2050 | CA  | PRO | A | 267 | 12.278 | 17.505 | 17.565 | 1.00 | 28.37 | C |
| ATOM | 2051 | C   | PRO | A | 267 | 13.148 | 17.313 | 16.360 | 1.00 | 28.01 | C |
| ATOM | 2052 | O   | PRO | A | 267 | 12.674 | 17.573 | 15.265 | 1.00 | 28.36 | O |
| ATOM | 2053 | CB  | PRO | A | 267 | 11.047 | 16.582 | 17.482 | 1.00 | 27.55 | C |
| ATOM | 2054 | CG  | PRO | A | 267 | 10.000 | 17.278 | 18.220 | 1.00 | 28.05 | C |
| ATOM | 2055 | CD  | PRO | A | 267 | 10.237 | 18.817 | 17.827 | 1.00 | 28.28 | C |
| ATOM | 2056 | N   | GLY | A | 268 | 14.392 | 16.878 | 16.562 | 1.00 | 27.37 | N |
| ATOM | 2057 | CA  | GLY | A | 268 | 15.273 | 16.605 | 15.453 | 1.00 | 25.78 | C |
| ATOM | 2058 | C   | GLY | A | 268 | 16.231 | 17.726 | 15.175 | 1.00 | 25.51 | C |
| ATOM | 2059 | O   | GLY | A | 268 | 17.237 | 17.508 | 14.519 | 1.00 | 26.07 | O |
| ATOM | 2060 | N   | ASP | A | 269 | 15.957 | 18.928 | 15.653 | 1.00 | 25.79 | N |
| ATOM | 2061 | CA  | ASP | A | 269 | 16.835 | 20.044 | 15.354 | 1.00 | 25.78 | C |
| ATOM | 2062 | C   | ASP | A | 269 | 17.996 | 20.091 | 16.377 | 1.00 | 26.28 | C |
| ATOM | 2063 | O   | ASP | A | 269 | 17.848 | 19.689 | 17.549 | 1.00 | 26.27 | O |
| ATOM | 2064 | CB  | ASP | A | 269 | 16.106 | 21.376 | 15.504 | 1.00 | 26.89 | C |
| ATOM | 2065 | CG  | ASP | A | 269 | 14.898 | 21.583 | 14.603 | 1.00 | 25.99 | C |
| ATOM | 2066 | OD1 | ASP | A | 269 | 14.745 | 20.966 | 13.562 | 1.00 | 28.50 | O |
| ATOM | 2067 | OD2 | ASP | A | 269 | 14.065 | 22.495 | 14.853 | 1.00 | 29.93 | O |
| ATOM | 2068 | N   | VAL | A | 270 | 19.128 | 20.632 | 15.937 | 1.00 | 26.28 | N |
| ATOM | 2069 | CA  | VAL | A | 270 | 20.291 | 20.847 | 16.775 | 1.00 | 26.03 | C |
| ATOM | 2070 | C   | VAL | A | 270 | 20.780 | 22.271 | 16.628 | 1.00 | 26.03 | C |
| ATOM | 2071 | O   | VAL | A | 270 | 21.123 | 22.727 | 15.547 | 1.00 | 25.72 | O |
| ATOM | 2072 | CB  | VAL | A | 270 | 21.414 | 19.938 | 16.381 | 1.00 | 25.76 | C |
| ATOM | 2073 | CG1 | VAL | A | 270 | 22.675 | 20.325 | 17.113 | 1.00 | 26.27 | C |
| ATOM | 2074 | CG2 | VAL | A | 270 | 21.060 | 18.546 | 16.735 | 1.00 | 25.93 | C |
| ATOM | 2075 | N   | LEU | A | 271 | 20.809 | 22.987 | 17.730 | 1.00 | 26.47 | N |
| ATOM | 2076 | CA  | LEU | A | 271 | 21.257 | 24.364 | 17.713 | 1.00 | 26.42 | C |
| ATOM | 2077 | C   | LEU | A | 271 | 22.673 | 24.422 | 18.228 | 1.00 | 27.12 | C |
| ATOM | 2078 | O   | LEU | A | 271 | 22.973 | 23.936 | 19.310 | 1.00 | 26.82 | O |
| ATOM | 2079 | CB  | LEU | A | 271 | 20.372 | 25.235 | 18.570 | 1.00 | 26.20 | C |
| ATOM | 2080 | CG  | LEU | A | 271 | 20.935 | 26.646 | 18.783 | 1.00 | 27.91 | C |
| ATOM | 2081 | CD1 | LEU | A | 271 | 20.962 | 27.396 | 17.500 | 1.00 | 27.86 | C |
| ATOM | 2082 | CD2 | LEU | A | 271 | 20.100 | 27.425 | 19.789 | 1.00 | 29.16 | C |
| ATOM | 2083 | N   | TYR | A | 272 | 23.563 | 24.980 | 17.423 | 1.00 | 27.82 | N |
| ATOM | 2084 | CA  | TYR | A | 272 | 24.913 | 25.201 | 17.873 | 1.00 | 27.79 | C |
| ATOM | 2085 | C   | TYR | A | 272 | 24.918 | 26.494 | 18.662 | 1.00 | 26.67 | C |
| ATOM | 2086 | O   | TYR | A | 272 | 24.660 | 27.528 | 18.117 | 1.00 | 27.22 | O |
| ATOM | 2087 | CB  | TYR | A | 272 | 25.898 | 25.325 | 16.693 | 1.00 | 27.26 | C |
| ATOM | 2088 | CG  | TYR | A | 272 | 27.296 | 25.785 | 17.124 | 1.00 | 28.18 | C |
| ATOM | 2089 | CD1 | TYR | A | 272 | 27.924 | 25.237 | 18.221 | 1.00 | 28.32 | C |
| ATOM | 2090 | CD2 | TYR | A | 272 | 27.973 | 26.784 | 16.435 | 1.00 | 29.06 | C |
| ATOM | 2091 | CE1 | TYR | A | 272 | 29.169 | 25.653 | 18.600 | 1.00 | 28.29 | C |
| ATOM | 2092 | CE2 | TYR | A | 272 | 29.232 | 27.188 | 16.805 | 1.00 | 27.19 | C |
| ATOM | 2093 | CZ  | TYR | A | 272 | 29.821 | 26.632 | 17.903 | 1.00 | 27.41 | C |
| ATOM | 2094 | OH  | TYR | A | 272 | 31.081 | 27.026 | 18.322 | 1.00 | 24.66 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2095 | N   | ILE | A | 273 | 25.237 | 26.418 | 19.934 | 1.00 | 26.87 | N |
| ATOM | 2096 | CA  | ILE | A | 273 | 25.381 | 27.591 | 20.810 | 1.00 | 26.89 | C |
| ATOM | 2097 | C   | ILE | A | 273 | 26.841 | 27.751 | 21.182 | 1.00 | 27.37 | C |
| ATOM | 2098 | O   | ILE | A | 273 | 27.359 | 27.049 | 22.056 | 1.00 | 27.62 | O |
| ATOM | 2099 | CB  | ILE | A | 273 | 24.647 | 27.422 | 22.085 | 1.00 | 26.74 | C |
| ATOM | 2100 | CG1 | ILE | A | 273 | 23.182 | 27.185 | 21.799 | 1.00 | 25.89 | C |
| ATOM | 2101 | CG2 | ILE | A | 273 | 24.852 | 28.675 | 22.941 | 1.00 | 26.79 | C |
| ATOM | 2102 | CD1 | ILE | A | 273 | 22.338 | 27.108 | 23.065 | 1.00 | 25.37 | C |
| ATOM | 2103 | N   | PRO | A | 274 | 27.491 | 28.681 | 20.515 | 1.00 | 27.39 | N |
| ATOM | 2104 | CA  | PRO | A | 274 | 28.923 | 28.871 | 20.601 | 1.00 | 27.76 | C |
| ATOM | 2105 | C   | PRO | A | 274 | 29.287 | 29.415 | 21.934 | 1.00 | 27.42 | C |
| ATOM | 2106 | O   | PRO | A | 274 | 28.483 | 30.135 | 22.518 | 1.00 | 26.71 | O |
| ATOM | 2107 | CB  | PRO | A | 274 | 29.250 | 29.840 | 19.426 | 1.00 | 27.60 | C |
| ATOM | 2108 | CG  | PRO | A | 274 | 27.980 | 30.107 | 18.741 | 1.00 | 28.16 | C |
| ATOM | 2109 | CD  | PRO | A | 274 | 26.876 | 29.504 | 19.497 | 1.00 | 28.21 | C |
| ATOM | 2110 | N   | MET | A | 275 | 30.467 | 29.017 | 22.394 | 1.00 | 27.88 | N |
| ATOM | 2111 | CA  | MET | A | 275 | 30.979 | 29.346 | 23.717 | 1.00 | 28.91 | C |
| ATOM | 2112 | C   | MET | A | 275 | 30.974 | 30.849 | 23.919 | 1.00 | 28.27 | C |
| ATOM | 2113 | O   | MET | A | 275 | 31.284 | 31.589 | 23.000 | 1.00 | 27.69 | O |
| ATOM | 2114 | CB  | MET | A | 275 | 32.365 | 28.808 | 23.869 | 1.00 | 29.00 | C |
| ATOM | 2115 | CG  | MET | A | 275 | 32.861 | 28.842 | 25.313 | 1.00 | 34.03 | C |
| ATOM | 2116 | SD  | MET | A | 275 | 34.499 | 28.084 | 25.455 | 1.00 | 39.22 | S |
| ATOM | 2117 | CE  | MET | A | 275 | 35.200 | 28.479 | 23.871 | 1.00 | 36.40 | C |
| ATOM | 2118 | N   | TYR | A | 276 | 30.531 | 31.294 | 25.086 | 1.00 | 27.79 | N |
| ATOM | 2119 | CA  | TYR | A | 276 | 30.472 | 32.746 | 25.389 | 1.00 | 29.16 | C |
| ATOM | 2120 | C   | TYR | A | 276 | 29.267 | 33.465 | 24.802 | 1.00 | 27.80 | C |
| ATOM | 2121 | O   | TYR | A | 276 | 29.076 | 34.609 | 25.107 | 1.00 | 28.35 | O |
| ATOM | 2122 | CB  | TYR | A | 276 | 31.779 | 33.506 | 24.974 | 1.00 | 29.63 | C |
| ATOM | 2123 | CG  | TYR | A | 276 | 32.918 | 33.207 | 25.897 | 1.00 | 34.37 | C |
| ATOM | 2124 | CD1 | TYR | A | 276 | 32.966 | 33.783 | 27.146 | 1.00 | 38.52 | C |
| ATOM | 2125 | CD2 | TYR | A | 276 | 33.934 | 32.306 | 25.547 | 1.00 | 39.45 | C |
| ATOM | 2126 | CE1 | TYR | A | 276 | 33.955 | 33.493 | 28.022 | 1.00 | 39.83 | C |
| ATOM | 2127 | CE2 | TYR | A | 276 | 34.965 | 32.015 | 26.449 | 1.00 | 42.05 | C |
| ATOM | 2128 | CZ  | TYR | A | 276 | 34.954 | 32.609 | 27.685 | 1.00 | 42.46 | C |
| ATOM | 2129 | OH  | TYR | A | 276 | 35.949 | 32.343 | 28.624 | 1.00 | 48.60 | O |
| ATOM | 2130 | N   | TRP | A | 277 | 28.468 | 32.830 | 23.951 | 1.00 | 27.45 | N |
| ATOM | 2131 | CA  | TRP | A | 277 | 27.271 | 33.485 | 23.419 | 1.00 | 26.19 | C |
| ATOM | 2132 | C   | TRP | A | 277 | 26.160 | 33.442 | 24.424 | 1.00 | 25.93 | C |
| ATOM | 2133 | O   | TRP | A | 277 | 25.882 | 32.409 | 24.973 | 1.00 | 26.84 | O |
| ATOM | 2134 | CB  | TRP | A | 277 | 26.796 | 32.826 | 22.130 | 1.00 | 26.07 | C |
| ATOM | 2135 | CG  | TRP | A | 277 | 27.525 | 33.276 | 20.957 | 1.00 | 24.33 | C |
| ATOM | 2136 | CD1 | TRP | A | 277 | 28.862 | 33.118 | 20.731 | 1.00 | 24.81 | C |
| ATOM | 2137 | CD2 | TRP | A | 277 | 26.995 | 33.935 | 19.821 | 1.00 | 23.88 | C |
| ATOM | 2138 | NE1 | TRP | A | 277 | 29.204 | 33.674 | 19.531 | 1.00 | 24.86 | N |
| ATOM | 2139 | CE2 | TRP | A | 277 | 28.073 | 34.182 | 18.944 | 1.00 | 24.16 | C |
| ATOM | 2140 | CE3 | TRP | A | 277 | 25.727 | 34.398 | 19.464 | 1.00 | 25.16 | C |
| ATOM | 2141 | CZ2 | TRP | A | 277 | 27.923 | 34.858 | 17.747 | 1.00 | 23.53 | C |
| ATOM | 2142 | CZ3 | TRP | A | 277 | 25.579 | 35.064 | 18.250 | 1.00 | 25.92 | C |
| ATOM | 2143 | CH2 | TRP | A | 277 | 26.679 | 35.292 | 17.414 | 1.00 | 24.81 | C |
| ATOM | 2144 | N   | TRP | A | 278 | 25.516 | 34.566 | 24.673 | 1.00 | 26.34 | N |
| ATOM | 2145 | CA  | TRP | A | 278 | 24.408 | 34.623 | 25.625 | 1.00 | 26.96 | C |
| ATOM | 2146 | C   | TRP | A | 278 | 23.229 | 33.847 | 25.050 | 1.00 | 27.33 | C |
| ATOM | 2147 | O   | TRP | A | 278 | 23.021 | 33.846 | 23.847 | 1.00 | 27.18 | O |
| ATOM | 2148 | CB  | TRP | A | 278 | 23.952 | 36.062 | 25.838 | 1.00 | 26.87 | C |
| ATOM | 2149 | CG  | TRP | A | 278 | 24.965 | 36.916 | 26.455 | 1.00 | 27.61 | C |
| ATOM | 2150 | CD1 | TRP | A | 278 | 25.997 | 37.558 | 25.833 | 1.00 | 28.27 | C |
| ATOM | 2151 | CD2 | TRP | A | 278 | 25.065 | 37.228 | 27.830 | 1.00 | 25.52 | C |
| ATOM | 2152 | NE1 | TRP | A | 278 | 26.731 | 38.261 | 26.753 | 1.00 | 28.77 | N |
| ATOM | 2153 | CE2 | TRP | A | 278 | 26.164 | 38.072 | 27.991 | 1.00 | 29.02 | C |
| ATOM | 2154 | CE3 | TRP | A | 278 | 24.303 | 36.915 | 28.942 | 1.00 | 26.86 | C |
| ATOM | 2155 | CZ2 | TRP | A | 278 | 26.541 | 38.563 | 29.224 | 1.00 | 28.96 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2156 | CZ3 | TRP | A | 278 | 24.676 | 37.402 | 30.157 | 1.00 | 29.86 | C |
| ATOM | 2157 | CH2 | TRP | A | 278 | 25.780 | 38.224 | 30.293 | 1.00 | 27.89 | C |
| ATOM | 2158 | N   | HIS | A | 279 | 22.455 | 33.193 | 25.890 | 1.00 | 27.47 | N |
| ATOM | 2159 | CA  | HIS | A | 279 | 21.263 | 32.554 | 25.380 | 1.00 | 28.50 | C |
| ATOM | 2160 | C   | HIS | A | 279 | 20.158 | 32.574 | 26.403 | 1.00 | 28.09 | C |
| ATOM | 2161 | O   | HIS | A | 279 | 20.420 | 32.445 | 27.584 | 1.00 | 29.26 | O |
| ATOM | 2162 | CB  | HIS | A | 279 | 21.528 | 31.112 | 24.899 | 1.00 | 28.46 | C |
| ATOM | 2163 | CG  | HIS | A | 279 | 22.339 | 30.278 | 25.838 | 1.00 | 30.29 | C |
| ATOM | 2164 | ND1 | HIS | A | 279 | 23.712 | 30.381 | 25.928 | 1.00 | 31.17 | N |
| ATOM | 2165 | CD2 | HIS | A | 279 | 21.984 | 29.270 | 26.673 | 1.00 | 31.89 | C |
| ATOM | 2166 | CE1 | HIS | A | 279 | 24.161 | 29.484 | 26.790 | 1.00 | 31.48 | C |
| ATOM | 2167 | NE2 | HIS | A | 279 | 23.136 | 28.810 | 27.271 | 1.00 | 30.92 | N |
| ATOM | 2168 | N   | HIS | A | 280 | 18.942 | 32.764 | 25.916 | 1.00 | 28.12 | N |
| ATOM | 2169 | CA  | HIS | A | 280 | 17.713 | 32.827 | 26.695 | 1.00 | 28.50 | C |
| ATOM | 2170 | C   | HIS | A | 280 | 16.884 | 31.731 | 26.071 | 1.00 | 28.78 | C |
| ATOM | 2171 | O   | HIS | A | 280 | 16.739 | 31.709 | 24.851 | 1.00 | 29.67 | O |
| ATOM | 2172 | CB  | HIS | A | 280 | 17.069 | 34.196 | 26.498 | 1.00 | 27.71 | C |
| ATOM | 2173 | CG  | HIS | A | 280 | 15.600 | 34.223 | 26.727 | 1.00 | 29.69 | C |
| ATOM | 2174 | ND1 | HIS | A | 280 | 15.021 | 34.905 | 27.782 | 1.00 | 31.66 | N |
| ATOM | 2175 | CD2 | HIS | A | 280 | 14.579 | 33.648 | 26.047 | 1.00 | 31.45 | C |
| ATOM | 2176 | CE1 | HIS | A | 280 | 13.710 | 34.743 | 27.738 | 1.00 | 30.66 | C |
| ATOM | 2177 | NE2 | HIS | A | 280 | 13.415 | 33.985 | 26.696 | 1.00 | 31.28 | N |
| ATOM | 2178 | N   | ILE | A | 281 | 16.346 | 30.814 | 26.860 | 1.00 | 29.23 | N |
| ATOM | 2179 | CA  | ILE | A | 281 | 15.651 | 29.652 | 26.294 | 1.00 | 29.56 | C |
| ATOM | 2180 | C   | ILE | A | 281 | 14.311 | 29.497 | 26.922 | 1.00 | 30.16 | C |
| ATOM | 2181 | O   | ILE | A | 281 | 14.190 | 29.517 | 28.135 | 1.00 | 30.14 | O |
| ATOM | 2182 | CB  | ILE | A | 281 | 16.478 | 28.409 | 26.516 | 1.00 | 29.69 | C |
| ATOM | 2183 | CG1 | ILE | A | 281 | 17.707 | 28.491 | 25.628 | 1.00 | 30.69 | C |
| ATOM | 2184 | CG2 | ILE | A | 281 | 15.686 | 27.119 | 26.172 | 1.00 | 28.22 | C |
| ATOM | 2185 | CD1 | ILE | A | 281 | 18.689 | 27.534 | 25.980 | 1.00 | 33.11 | C |
| ATOM | 2186 | N   | GLU | A | 282 | 13.280 | 29.380 | 26.103 | 1.00 | 31.22 | N |
| ATOM | 2187 | CA  | GLU | A | 282 | 11.931 | 29.278 | 26.665 | 1.00 | 31.99 | C |
| ATOM | 2188 | C   | GLU | A | 282 | 11.123 | 28.182 | 26.007 | 1.00 | 31.79 | C |
| ATOM | 2189 | O   | GLU | A | 282 | 11.131 | 28.021 | 24.806 | 1.00 | 32.77 | O |
| ATOM | 2190 | CB  | GLU | A | 282 | 11.200 | 30.638 | 26.618 | 1.00 | 32.16 | C |
| ATOM | 2191 | CG  | GLU | A | 282 | 11.017 | 31.265 | 25.253 | 1.00 | 33.49 | C |
| ATOM | 2192 | CD  | GLU | A | 282 | 10.378 | 32.663 | 25.313 | 1.00 | 36.22 | C |
| ATOM | 2193 | OE1 | GLU | A | 282 | 10.879 | 33.552 | 26.043 | 1.00 | 38.20 | O |
| ATOM | 2194 | OE2 | GLU | A | 282 | 9.380  | 32.898 | 24.603 | 1.00 | 38.15 | O |
| ATOM | 2195 | N   | SER | A | 283 | 10.454 | 27.392 | 26.827 | 1.00 | 31.81 | N |
| ATOM | 2196 | CA  | SER | A | 283 | 9.592  | 26.333 | 26.331 | 1.00 | 30.79 | C |
| ATOM | 2197 | C   | SER | A | 283 | 8.245  | 26.975 | 25.950 | 1.00 | 30.98 | C |
| ATOM | 2198 | O   | SER | A | 283 | 7.635  | 27.640 | 26.780 | 1.00 | 30.36 | O |
| ATOM | 2199 | CB  | SER | A | 283 | 9.430  | 25.305 | 27.424 | 1.00 | 30.62 | C |
| ATOM | 2200 | OG  | SER | A | 283 | 10.586 | 24.463 | 27.496 | 1.00 | 29.45 | O |
| ATOM | 2201 | N   | LEU | A | 284 | 7.776  | 26.790 | 24.709 | 1.00 | 31.06 | N |
| ATOM | 2202 | CA  | LEU | A | 284 | 6.587  | 27.504 | 24.270 | 1.00 | 31.43 | C |
| ATOM | 2203 | C   | LEU | A | 284 | 5.398  | 27.390 | 25.204 | 1.00 | 31.82 | C |
| ATOM | 2204 | O   | LEU | A | 284 | 5.137  | 26.333 | 25.776 | 1.00 | 31.15 | O |
| ATOM | 2205 | CB  | LEU | A | 284 | 6.156  | 27.098 | 22.895 | 1.00 | 31.75 | C |
| ATOM | 2206 | CG  | LEU | A | 284 | 7.223  | 27.187 | 21.829 | 1.00 | 33.11 | C |
| ATOM | 2207 | CD1 | LEU | A | 284 | 6.571  | 27.388 | 20.478 | 1.00 | 33.62 | C |
| ATOM | 2208 | CD2 | LEU | A | 284 | 8.170  | 28.270 | 22.142 | 1.00 | 32.91 | C |
| ATOM | 2209 | N   | LEU | A | 285 | 4.701  | 28.512 | 25.355 | 1.00 | 32.74 | N |
| ATOM | 2210 | CA  | LEU | A | 285 | 3.481  | 28.564 | 26.147 | 1.00 | 34.35 | C |
| ATOM | 2211 | C   | LEU | A | 285 | 2.502  | 27.591 | 25.540 | 1.00 | 34.74 | C |
| ATOM | 2212 | O   | LEU | A | 285 | 2.375  | 27.510 | 24.332 | 1.00 | 34.70 | O |
| ATOM | 2213 | CB  | LEU | A | 285 | 2.863  | 29.946 | 26.094 | 1.00 | 34.26 | C |
| ATOM | 2214 | CG  | LEU | A | 285 | 3.729  | 31.060 | 26.638 | 1.00 | 34.74 | C |
| ATOM | 2215 | CD1 | LEU | A | 285 | 3.183  | 32.369 | 26.160 | 1.00 | 34.14 | C |
| ATOM | 2216 | CD2 | LEU | A | 285 | 3.780  | 30.970 | 28.136 | 1.00 | 34.97 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2217 | N   | ASN | A | 286 | 1.838  | 26.829 | 26.380 | 1.00 | 35.89 | N |
| ATOM | 2218 | CA  | ASN | A | 286 | 0.841  | 25.863 | 25.896 | 1.00 | 37.12 | C |
| ATOM | 2219 | C   | ASN | A | 286 | 1.363  | 24.809 | 24.909 | 1.00 | 36.14 | C |
| ATOM | 2220 | O   | ASN | A | 286 | 0.600  | 24.306 | 24.108 | 1.00 | 35.85 | O |
| ATOM | 2221 | CB  | ASN | A | 286 | -0.336 | 26.635 | 25.274 | 1.00 | 37.80 | C |
| ATOM | 2222 | CG  | ASN | A | 286 | -0.882 | 27.690 | 26.219 | 1.00 | 42.02 | C |
| ATOM | 2223 | OD1 | ASN | A | 286 | -1.326 | 27.365 | 27.326 | 1.00 | 47.86 | O |
| ATOM | 2224 | ND2 | ASN | A | 286 | -0.809 | 28.965 | 25.817 | 1.00 | 46.67 | N |
| ATOM | 2225 | N   | GLY | A | 287 | 2.653  | 24.478 | 24.974 | 1.00 | 35.43 | N |
| ATOM | 2226 | CA  | GLY | A | 287 | 3.262  | 23.539 | 24.057 | 1.00 | 34.11 | C |
| ATOM | 2227 | C   | GLY | A | 287 | 3.569  | 22.202 | 24.666 | 1.00 | 34.02 | C |
| ATOM | 2228 | O   | GLY | A | 287 | 4.073  | 21.317 | 23.977 | 1.00 | 34.98 | O |
| ATOM | 2229 | N   | GLY | A | 288 | 3.242  | 22.023 | 25.944 | 1.00 | 33.71 | N |
| ATOM | 2230 | CA  | GLY | A | 288 | 3.476  | 20.759 | 26.616 | 1.00 | 33.00 | C |
| ATOM | 2231 | C   | GLY | A | 288 | 4.908  | 20.692 | 27.107 | 1.00 | 33.19 | C |
| ATOM | 2232 | O   | GLY | A | 288 | 5.625  | 21.681 | 26.989 | 1.00 | 33.40 | O |
| ATOM | 2233 | N   | ILE | A | 289 | 5.337  | 19.540 | 27.621 | 1.00 | 32.87 | N |
| ATOM | 2234 | CA  | ILE | A | 289 | 6.647  | 19.425 | 28.195 | 1.00 | 33.57 | C |
| ATOM | 2235 | C   | ILE | A | 289 | 7.695  | 19.434 | 27.118 | 1.00 | 33.13 | C |
| ATOM | 2236 | O   | ILE | A | 289 | 7.454  | 19.023 | 25.995 | 1.00 | 34.41 | O |
| ATOM | 2237 | CB  | ILE | A | 289 | 6.809  | 18.137 | 29.006 | 1.00 | 34.25 | C |
| ATOM | 2238 | CG1 | ILE | A | 289 | 6.789  | 16.920 | 28.102 | 1.00 | 36.60 | C |
| ATOM | 2239 | CG2 | ILE | A | 289 | 5.746  | 18.005 | 30.113 | 1.00 | 34.91 | C |
| ATOM | 2240 | CD1 | ILE | A | 289 | 7.271  | 15.659 | 28.834 | 1.00 | 38.16 | C |
| ATOM | 2241 | N   | THR | A | 290 | 8.891  | 19.868 | 27.465 | 1.00 | 31.68 | N |
| ATOM | 2242 | CA  | THR | A | 290 | 9.956  | 19.853 | 26.498 | 1.00 | 29.79 | C |
| ATOM | 2243 | C   | THR | A | 290 | 11.054 | 18.938 | 26.958 | 1.00 | 27.97 | C |
| ATOM | 2244 | O   | THR | A | 290 | 11.256 | 18.739 | 28.133 | 1.00 | 26.58 | O |
| ATOM | 2245 | CB  | THR | A | 290 | 10.526 | 21.278 | 26.305 | 1.00 | 30.77 | C |
| ATOM | 2246 | OG1 | THR | A | 290 | 10.957 | 21.827 | 27.554 | 1.00 | 27.89 | O |
| ATOM | 2247 | CG2 | THR | A | 290 | 9.458  | 22.243 | 25.789 | 1.00 | 30.82 | C |
| ATOM | 2248 | N   | ILE | A | 291 | 11.787 | 18.395 | 26.021 | 1.00 | 26.96 | N |
| ATOM | 2249 | CA  | ILE | A | 291 | 12.910 | 17.594 | 26.383 | 1.00 | 27.83 | C |
| ATOM | 2250 | C   | ILE | A | 291 | 14.059 | 17.952 | 25.493 | 1.00 | 27.31 | C |
| ATOM | 2251 | O   | ILE | A | 291 | 13.880 | 18.028 | 24.289 | 1.00 | 27.83 | O |
| ATOM | 2252 | CB  | ILE | A | 291 | 12.596 | 16.104 | 26.195 | 1.00 | 28.72 | C |
| ATOM | 2253 | CG1 | ILE | A | 291 | 11.480 | 15.671 | 27.140 | 1.00 | 29.09 | C |
| ATOM | 2254 | CG2 | ILE | A | 291 | 13.865 | 15.278 | 26.438 | 1.00 | 28.55 | C |
| ATOM | 2255 | CD1 | ILE | A | 291 | 11.115 | 14.232 | 26.986 | 1.00 | 30.86 | C |
| ATOM | 2256 | N   | THR | A | 292 | 15.240 | 18.093 | 26.074 | 1.00 | 26.63 | N |
| ATOM | 2257 | CA  | THR | A | 292 | 16.415 | 18.444 | 25.333 | 1.00 | 26.88 | C |
| ATOM | 2258 | C   | THR | A | 292 | 17.587 | 17.724 | 25.915 | 1.00 | 26.52 | C |
| ATOM | 2259 | O   | THR | A | 292 | 17.631 | 17.524 | 27.102 | 1.00 | 26.40 | O |
| ATOM | 2260 | CB  | THR | A | 292 | 16.753 | 19.971 | 25.532 | 1.00 | 27.41 | C |
| ATOM | 2261 | OG1 | THR | A | 292 | 15.652 | 20.841 | 25.187 | 1.00 | 28.64 | O |
| ATOM | 2262 | CG2 | THR | A | 292 | 17.852 | 20.398 | 24.592 | 1.00 | 28.03 | C |
| ATOM | 2263 | N   | VAL | A | 293 | 18.577 | 17.414 | 25.093 | 1.00 | 26.32 | N |
| ATOM | 2264 | CA  | VAL | A | 293 | 19.834 | 16.896 | 25.585 | 1.00 | 26.86 | C |
| ATOM | 2265 | C   | VAL | A | 293 | 20.964 | 17.718 | 24.978 | 1.00 | 27.24 | C |
| ATOM | 2266 | O   | VAL | A | 293 | 21.011 | 17.892 | 23.757 | 1.00 | 26.60 | O |
| ATOM | 2267 | CB  | VAL | A | 293 | 20.029 | 15.422 | 25.226 | 1.00 | 27.56 | C |
| ATOM | 2268 | CG1 | VAL | A | 293 | 21.472 | 15.004 | 25.411 | 1.00 | 27.42 | C |
| ATOM | 2269 | CG2 | VAL | A | 293 | 19.138 | 14.546 | 26.126 | 1.00 | 29.64 | C |
| ATOM | 2270 | N   | ASN | A | 294 | 21.849 | 18.278 | 25.814 | 1.00 | 27.26 | N |
| ATOM | 2271 | CA  | ASN | A | 294 | 22.960 | 19.055 | 25.258 | 1.00 | 27.81 | C |
| ATOM | 2272 | C   | ASN | A | 294 | 24.253 | 18.268 | 25.281 | 1.00 | 27.79 | C |
| ATOM | 2273 | O   | ASN | A | 294 | 24.338 | 17.177 | 25.883 | 1.00 | 28.63 | O |
| ATOM | 2274 | CB  | ASN | A | 294 | 23.118 | 20.446 | 25.881 | 1.00 | 27.69 | C |
| ATOM | 2275 | CG  | ASN | A | 294 | 23.703 | 20.405 | 27.287 | 1.00 | 30.08 | C |
| ATOM | 2276 | OD1 | ASN | A | 294 | 24.309 | 19.397 | 27.677 | 1.00 | 29.80 | O |
| ATOM | 2277 | ND2 | ASN | A | 294 | 23.513 | 21.506 | 28.064 | 1.00 | 28.15 | N |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2278 | N   | PHE | A | 295 | 25.235 | 18.816 | 24.576 | 1.00 | 27.46 | N |
| ATOM | 2279 | CA  | PHE | A | 295 | 26.548 | 18.219 | 24.428 | 1.00 | 27.53 | C |
| ATOM | 2280 | C   | PHE | A | 295 | 27.543 | 19.352 | 24.675 | 1.00 | 28.01 | C |
| ATOM | 2281 | O   | PHE | A | 295 | 27.720 | 20.239 | 23.811 | 1.00 | 28.48 | O |
| ATOM | 2282 | CB  | PHE | A | 295 | 26.756 | 17.703 | 23.009 | 1.00 | 27.33 | C |
| ATOM | 2283 | CG  | PHE | A | 295 | 25.955 | 16.487 | 22.658 | 1.00 | 27.87 | C |
| ATOM | 2284 | CD1 | PHE | A | 295 | 24.586 | 16.560 | 22.496 | 1.00 | 27.75 | C |
| ATOM | 2285 | CD2 | PHE | A | 295 | 26.581 | 15.287 | 22.426 | 1.00 | 26.57 | C |
| ATOM | 2286 | CE1 | PHE | A | 295 | 23.892 | 15.466 | 22.147 | 1.00 | 28.45 | C |
| ATOM | 2287 | CE2 | PHE | A | 295 | 25.869 | 14.187 | 22.095 | 1.00 | 27.40 | C |
| ATOM | 2288 | CZ  | PHE | A | 295 | 24.541 | 14.262 | 21.952 | 1.00 | 27.57 | C |
| ATOM | 2289 | N   | TRP | A | 296 | 28.166 | 19.346 | 25.852 | 1.00 | 28.46 | N |
| ATOM | 2290 | CA  | TRP | A | 296 | 29.097 | 20.402 | 26.249 | 1.00 | 29.05 | C |
| ATOM | 2291 | C   | TRP | A | 296 | 30.545 | 19.950 | 26.077 | 1.00 | 29.39 | C |
| ATOM | 2292 | O   | TRP | A | 296 | 30.981 | 18.942 | 26.663 | 1.00 | 29.90 | O |
| ATOM | 2293 | CB  | TRP | A | 296 | 28.850 | 20.825 | 27.696 | 1.00 | 29.23 | C |
| ATOM | 2294 | CG  | TRP | A | 296 | 27.917 | 21.982 | 27.908 | 1.00 | 31.21 | C |
| ATOM | 2295 | CD1 | TRP | A | 296 | 27.805 | 23.080 | 27.135 | 1.00 | 33.45 | C |
| ATOM | 2296 | CD2 | TRP | A | 296 | 26.995 | 22.171 | 28.996 | 1.00 | 33.70 | C |
| ATOM | 2297 | NE1 | TRP | A | 296 | 26.864 | 23.941 | 27.651 | 1.00 | 33.91 | N |
| ATOM | 2298 | CE2 | TRP | A | 296 | 26.344 | 23.403 | 28.787 | 1.00 | 33.49 | C |
| ATOM | 2299 | CE3 | TRP | A | 296 | 26.638 | 21.414 | 30.113 | 1.00 | 36.30 | C |
| ATOM | 2300 | CZ2 | TRP | A | 296 | 25.377 | 23.902 | 29.642 | 1.00 | 35.59 | C |
| ATOM | 2301 | CZ3 | TRP | A | 296 | 25.643 | 21.899 | 30.967 | 1.00 | 37.80 | C |
| ATOM | 2302 | CH2 | TRP | A | 296 | 25.034 | 23.141 | 30.727 | 1.00 | 37.39 | C |
| ATOM | 2303 | N   | TYR | A | 297 | 31.288 | 20.720 | 25.292 | 1.00 | 29.87 | N |
| ATOM | 2304 | CA  | TYR | A | 297 | 32.693 | 20.472 | 25.017 | 1.00 | 30.43 | C |
| ATOM | 2305 | C   | TYR | A | 297 | 33.548 | 21.629 | 25.518 | 1.00 | 30.98 | C |
| ATOM | 2306 | O   | TYR | A | 297 | 33.167 | 22.765 | 25.387 | 1.00 | 29.50 | O |
| ATOM | 2307 | CB  | TYR | A | 297 | 32.909 | 20.334 | 23.502 | 1.00 | 30.36 | C |
| ATOM | 2308 | CG  | TYR | A | 297 | 32.304 | 19.083 | 22.919 | 1.00 | 30.07 | C |
| ATOM | 2309 | CD1 | TYR | A | 297 | 30.946 | 19.012 | 22.627 | 1.00 | 29.74 | C |
| ATOM | 2310 | CD2 | TYR | A | 297 | 33.083 | 17.960 | 22.687 | 1.00 | 28.56 | C |
| ATOM | 2311 | CE1 | TYR | A | 297 | 30.397 | 17.859 | 22.105 | 1.00 | 28.46 | C |
| ATOM | 2312 | CE2 | TYR | A | 297 | 32.546 | 16.800 | 22.213 | 1.00 | 27.77 | C |
| ATOM | 2313 | CZ  | TYR | A | 297 | 31.202 | 16.758 | 21.913 | 1.00 | 28.10 | C |
| ATOM | 2314 | OH  | TYR | A | 297 | 30.654 | 15.613 | 21.438 | 1.00 | 27.72 | O |
| ATOM | 2315 | N   | LYS | A | 298 | 34.723 | 21.325 | 26.060 | 1.00 | 32.77 | N |
| ATOM | 2316 | CA  | LYS | A | 298 | 35.671 | 22.349 | 26.470 | 1.00 | 34.43 | C |
| ATOM | 2317 | C   | LYS | A | 298 | 36.126 | 23.014 | 25.216 | 1.00 | 34.91 | C |
| ATOM | 2318 | O   | LYS | A | 298 | 36.236 | 22.373 | 24.194 | 1.00 | 35.28 | O |
| ATOM | 2319 | CB  | LYS | A | 298 | 36.865 | 21.749 | 27.221 | 1.00 | 35.25 | C |
| ATOM | 2320 | CG  | LYS | A | 298 | 36.595 | 21.446 | 28.725 | 1.00 | 38.48 | C |
| ATOM | 2321 | CD  | LYS | A | 298 | 37.834 | 20.990 | 29.532 | 1.00 | 42.40 | C |
| ATOM | 2322 | CE  | LYS | A | 298 | 37.429 | 20.600 | 30.991 | 1.00 | 45.34 | C |
| ATOM | 2323 | NZ  | LYS | A | 298 | 38.515 | 19.883 | 31.770 | 1.00 | 49.07 | N |
| ATOM | 2324 | N   | GLY | A | 299 | 36.384 | 24.305 | 25.267 | 1.00 | 36.67 | N |
| ATOM | 2325 | CA  | GLY | A | 299 | 36.837 | 24.998 | 24.080 | 1.00 | 38.01 | C |
| ATOM | 2326 | C   | GLY | A | 299 | 38.249 | 24.618 | 23.689 | 1.00 | 39.33 | C |
| ATOM | 2327 | O   | GLY | A | 299 | 38.965 | 23.987 | 24.437 | 1.00 | 39.19 | O |
| ATOM | 2328 | N   | ALA | A | 300 | 38.644 | 25.017 | 22.498 | 1.00 | 41.68 | N |
| ATOM | 2329 | CA  | ALA | A | 300 | 40.014 | 24.844 | 22.048 | 1.00 | 43.93 | C |
| ATOM | 2330 | C   | ALA | A | 300 | 40.964 | 25.618 | 22.940 | 1.00 | 45.88 | C |
| ATOM | 2331 | O   | ALA | A | 300 | 40.558 | 26.437 | 23.741 | 1.00 | 46.12 | O |
| ATOM | 2332 | CB  | ALA | A | 300 | 40.148 | 25.343 | 20.639 | 1.00 | 43.86 | C |
| ATOM | 2333 | N   | PRO | A | 301 | 42.254 | 25.393 | 22.773 | 1.00 | 49.19 | N |
| ATOM | 2334 | CA  | PRO | A | 301 | 43.251 | 26.084 | 23.605 | 1.00 | 50.79 | C |
| ATOM | 2335 | C   | PRO | A | 301 | 43.465 | 27.525 | 23.204 | 1.00 | 52.01 | C |
| ATOM | 2336 | O   | PRO | A | 301 | 43.302 | 27.869 | 22.041 | 1.00 | 52.73 | O |
| ATOM | 2337 | CB  | PRO | A | 301 | 44.534 | 25.325 | 23.303 | 1.00 | 50.51 | C |
| ATOM | 2338 | CG  | PRO | A | 301 | 44.357 | 24.908 | 21.884 | 1.00 | 50.75 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2339 | CD  | PRO | A | 301 | 42.890 | 24.521 | 21.766 | 1.00 | 49.57 | C |
| ATOM | 2340 | N   | THR | A | 302 | 43.831 | 28.346 | 24.169 | 1.00 | 53.76 | N |
| ATOM | 2341 | CA  | THR | A | 302 | 44.173 | 29.736 | 23.928 | 1.00 | 55.20 | C |
| ATOM | 2342 | C   | THR | A | 302 | 45.563 | 29.720 | 23.307 | 1.00 | 56.14 | C |
| ATOM | 2343 | O   | THR | A | 302 | 46.504 | 29.273 | 23.980 | 1.00 | 56.50 | O |
| ATOM | 2344 | CB  | THR | A | 302 | 44.249 | 30.449 | 25.274 | 1.00 | 55.30 | C |
| ATOM | 2345 | OG1 | THR | A | 302 | 42.959 | 30.448 | 25.909 | 1.00 | 57.92 | O |
| ATOM | 2346 | CG2 | THR | A | 302 | 44.552 | 31.886 | 25.090 | 1.00 | 56.33 | C |
| ATOM | 2347 | N   | PRO | A | 303 | 45.743 | 30.239 | 22.086 | 1.00 | 56.60 | N |
| ATOM | 2348 | CA  | PRO | A | 303 | 47.057 | 30.145 | 21.427 | 1.00 | 56.45 | C |
| ATOM | 2349 | C   | PRO | A | 303 | 48.168 | 30.743 | 22.280 | 1.00 | 56.31 | C |
| ATOM | 2350 | O   | PRO | A | 303 | 47.845 | 31.449 | 23.235 | 1.00 | 56.29 | O |
| ATOM | 2351 | CB  | PRO | A | 303 | 46.883 | 30.989 | 20.168 | 1.00 | 56.55 | C |
| ATOM | 2352 | CG  | PRO | A | 303 | 45.418 | 31.007 | 19.927 | 1.00 | 56.34 | C |
| ATOM | 2353 | CD  | PRO | A | 303 | 44.812 | 31.082 | 21.309 | 1.00 | 56.48 | C |
| ATOM | 2354 | N   | GLU | A | 307 | 46.896 | 37.001 | 18.664 | 1.00 | 61.01 | N |
| ATOM | 2355 | CA  | GLU | A | 307 | 46.873 | 37.991 | 17.591 | 1.00 | 61.50 | C |
| ATOM | 2356 | C   | GLU | A | 307 | 45.852 | 39.079 | 17.834 | 1.00 | 60.73 | C |
| ATOM | 2357 | O   | GLU | A | 307 | 44.755 | 38.828 | 18.308 | 1.00 | 61.45 | O |
| ATOM | 2358 | CB  | GLU | A | 307 | 46.614 | 37.356 | 16.205 | 1.00 | 62.21 | C |
| ATOM | 2359 | CG  | GLU | A | 307 | 46.871 | 38.339 | 15.045 | 1.00 | 63.86 | C |
| ATOM | 2360 | CD  | GLU | A | 307 | 46.898 | 37.697 | 13.665 | 1.00 | 65.26 | C |
| ATOM | 2361 | OE1 | GLU | A | 307 | 46.468 | 36.535 | 13.516 | 1.00 | 65.73 | O |
| ATOM | 2362 | OE2 | GLU | A | 307 | 47.342 | 38.382 | 12.718 | 1.00 | 67.94 | O |
| ATOM | 2363 | N   | TYR | A | 308 | 46.237 | 40.302 | 17.513 | 1.00 | 59.88 | N |
| ATOM | 2364 | CA  | TYR | A | 308 | 45.349 | 41.441 | 17.639 | 1.00 | 59.19 | C |
| ATOM | 2365 | C   | TYR | A | 308 | 44.706 | 41.622 | 16.279 | 1.00 | 58.70 | C |
| ATOM | 2366 | O   | TYR | A | 308 | 45.224 | 41.120 | 15.273 | 1.00 | 59.29 | O |
| ATOM | 2367 | CB  | TYR | A | 308 | 46.133 | 42.665 | 18.095 | 1.00 | 59.18 | C |
| ATOM | 2368 | CG  | TYR | A | 308 | 46.677 | 42.418 | 19.478 | 1.00 | 59.73 | C |
| ATOM | 2369 | CD1 | TYR | A | 308 | 45.904 | 42.708 | 20.605 | 1.00 | 59.74 | C |
| ATOM | 2370 | CD2 | TYR | A | 308 | 47.912 | 41.801 | 19.665 | 1.00 | 59.94 | C |
| ATOM | 2371 | CE1 | TYR | A | 308 | 46.357 | 42.438 | 21.869 | 1.00 | 59.94 | C |
| ATOM | 2372 | CE2 | TYR | A | 308 | 48.377 | 41.519 | 20.933 | 1.00 | 61.17 | C |
| ATOM | 2373 | CZ  | TYR | A | 308 | 47.592 | 41.843 | 22.038 | 1.00 | 61.68 | C |
| ATOM | 2374 | OH  | TYR | A | 308 | 48.032 | 41.579 | 23.316 | 1.00 | 63.29 | O |
| ATOM | 2375 | N   | PRO | A | 309 | 43.541 | 42.258 | 16.233 | 1.00 | 57.37 | N |
| ATOM | 2376 | CA  | PRO | A | 309 | 42.849 | 42.815 | 17.411 | 1.00 | 55.72 | C |
| ATOM | 2377 | C   | PRO | A | 309 | 42.113 | 41.742 | 18.225 | 1.00 | 52.85 | C |
| ATOM | 2378 | O   | PRO | A | 309 | 41.627 | 40.815 | 17.613 | 1.00 | 53.22 | O |
| ATOM | 2379 | CB  | PRO | A | 309 | 41.823 | 43.755 | 16.777 | 1.00 | 56.31 | C |
| ATOM | 2380 | CG  | PRO | A | 309 | 41.512 | 43.113 | 15.410 | 1.00 | 57.04 | C |
| ATOM | 2381 | CD  | PRO | A | 309 | 42.774 | 42.431 | 14.984 | 1.00 | 57.43 | C |
| ATOM | 2382 | N   | LEU | A | 310 | 41.998 | 41.879 | 19.544 | 1.00 | 49.67 | N |
| ATOM | 2383 | CA  | LEU | A | 310 | 41.368 | 40.825 | 20.363 | 1.00 | 47.23 | C |
| ATOM | 2384 | C   | LEU | A | 310 | 39.870 | 40.656 | 20.128 | 1.00 | 45.07 | C |
| ATOM | 2385 | O   | LEU | A | 310 | 39.131 | 41.635 | 19.956 | 1.00 | 45.94 | O |
| ATOM | 2386 | CB  | LEU | A | 310 | 41.568 | 41.109 | 21.837 | 1.00 | 46.99 | C |
| ATOM | 2387 | CG  | LEU | A | 310 | 42.579 | 40.351 | 22.706 | 1.00 | 46.52 | C |
| ATOM | 2388 | CD1 | LEU | A | 310 | 43.856 | 40.028 | 22.048 | 1.00 | 45.64 | C |
| ATOM | 2389 | CD2 | LEU | A | 310 | 42.840 | 41.179 | 23.975 | 1.00 | 46.57 | C |
| ATOM | 2390 | N   | LYS | A | 311 | 39.408 | 39.414 | 20.139 | 1.00 | 41.52 | N |
| ATOM | 2391 | CA  | LYS | A | 311 | 37.987 | 39.155 | 20.003 | 1.00 | 38.55 | C |
| ATOM | 2392 | C   | LYS | A | 311 | 37.179 | 39.463 | 21.276 | 1.00 | 35.80 | C |
| ATOM | 2393 | O   | LYS | A | 311 | 37.664 | 39.425 | 22.400 | 1.00 | 34.43 | O |
| ATOM | 2394 | CB  | LYS | A | 311 | 37.760 | 37.727 | 19.553 | 1.00 | 39.46 | C |
| ATOM | 2395 | N   | ALA | A | 312 | 35.920 | 39.786 | 21.076 | 1.00 | 32.82 | N |
| ATOM | 2396 | CA  | ALA | A | 312 | 35.055 | 40.081 | 22.185 | 1.00 | 30.91 | C |
| ATOM | 2397 | C   | ALA | A | 312 | 35.152 | 39.033 | 23.279 | 1.00 | 30.00 | C |
| ATOM | 2398 | O   | ALA | A | 312 | 35.231 | 39.382 | 24.442 | 1.00 | 28.68 | O |
| ATOM | 2399 | CB  | ALA | A | 312 | 33.625 | 40.234 | 21.707 | 1.00 | 30.07 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2400 | N   | HIS | A | 313 | 35.148 | 37.753 | 22.916 | 1.00 | 29.85 | N |
| ATOM | 2401 | CA  | HIS | A | 313 | 35.125 | 36.727 | 23.931 | 1.00 | 30.47 | C |
| ATOM | 2402 | C   | HIS | A | 313 | 36.410 | 36.710 | 24.689 | 1.00 | 29.99 | C |
| ATOM | 2403 | O   | HIS | A | 313 | 36.439 | 36.320 | 25.846 | 1.00 | 29.25 | O |
| ATOM | 2404 | CB  | HIS | A | 313 | 34.787 | 35.331 | 23.392 | 1.00 | 31.64 | C |
| ATOM | 2405 | CG  | HIS | A | 313 | 35.860 | 34.714 | 22.566 | 1.00 | 35.54 | C |
| ATOM | 2406 | ND1 | HIS | A | 313 | 35.987 | 34.950 | 21.208 | 1.00 | 41.10 | N |
| ATOM | 2407 | CD2 | HIS | A | 313 | 36.844 | 33.846 | 22.891 | 1.00 | 40.77 | C |
| ATOM | 2408 | CE1 | HIS | A | 313 | 37.047 | 34.303 | 20.750 | 1.00 | 40.02 | C |
| ATOM | 2409 | NE2 | HIS | A | 313 | 37.567 | 33.603 | 21.743 | 1.00 | 41.82 | N |
| ATOM | 2410 | N   | GLN | A | 314 | 37.482 | 37.137 | 24.056 | 1.00 | 29.68 | N |
| ATOM | 2411 | CA  | GLN | A | 314 | 38.754 | 37.185 | 24.751 | 1.00 | 29.77 | C |
| ATOM | 2412 | C   | GLN | A | 314 | 38.729 | 38.294 | 25.817 | 1.00 | 30.57 | C |
| ATOM | 2413 | O   | GLN | A | 314 | 39.222 | 38.120 | 26.956 | 1.00 | 29.69 | O |
| ATOM | 2414 | CB  | GLN | A | 314 | 39.893 | 37.401 | 23.743 | 1.00 | 30.02 | C |
| ATOM | 2415 | CG  | GLN | A | 314 | 40.111 | 36.182 | 22.786 | 1.00 | 29.84 | C |
| ATOM | 2416 | CD  | GLN | A | 314 | 41.126 | 36.437 | 21.687 | 1.00 | 31.76 | C |
| ATOM | 2417 | OE1 | GLN | A | 314 | 40.982 | 37.377 | 20.885 | 1.00 | 32.81 | O |
| ATOM | 2418 | NE2 | GLN | A | 314 | 42.160 | 35.594 | 21.637 | 1.00 | 34.23 | N |
| ATOM | 2419 | N   | LYS | A | 315 | 38.111 | 39.421 | 25.471 | 1.00 | 30.44 | N |
| ATOM | 2420 | CA  | LYS | A | 315 | 38.026 | 40.491 | 26.431 | 1.00 | 31.27 | C |
| ATOM | 2421 | C   | LYS | A | 315 | 37.192 | 40.023 | 27.635 | 1.00 | 30.75 | C |
| ATOM | 2422 | O   | LYS | A | 315 | 37.511 | 40.373 | 28.784 | 1.00 | 29.60 | O |
| ATOM | 2423 | CB  | LYS | A | 315 | 37.461 | 41.752 | 25.808 | 1.00 | 31.76 | C |
| ATOM | 2424 | CG  | LYS | A | 315 | 38.483 | 42.491 | 24.982 | 1.00 | 33.90 | C |
| ATOM | 2425 | CD  | LYS | A | 315 | 37.902 | 43.711 | 24.329 | 1.00 | 37.97 | C |
| ATOM | 2426 | CE  | LYS | A | 315 | 38.911 | 44.380 | 23.419 | 1.00 | 41.69 | C |
| ATOM | 2427 | NZ  | LYS | A | 315 | 38.264 | 45.411 | 22.536 | 1.00 | 44.93 | N |
| ATOM | 2428 | N   | VAL | A | 316 | 36.163 | 39.216 | 27.362 | 1.00 | 29.26 | N |
| ATOM | 2429 | CA  | VAL | A | 316 | 35.318 | 38.731 | 28.422 | 1.00 | 29.23 | C |
| ATOM | 2430 | C   | VAL | A | 316 | 36.152 | 37.841 | 29.339 | 1.00 | 29.87 | C |
| ATOM | 2431 | O   | VAL | A | 316 | 36.075 | 37.926 | 30.584 | 1.00 | 30.33 | O |
| ATOM | 2432 | CB  | VAL | A | 316 | 34.079 | 37.973 | 27.900 | 1.00 | 28.68 | C |
| ATOM | 2433 | CG1 | VAL | A | 316 | 33.306 | 37.376 | 29.037 | 1.00 | 28.32 | C |
| ATOM | 2434 | CG2 | VAL | A | 316 | 33.144 | 38.887 | 27.136 | 1.00 | 28.57 | C |
| ATOM | 2435 | N   | ALA | A | 317 | 36.976 | 37.007 | 28.728 | 1.00 | 29.36 | N |
| ATOM | 2436 | CA  | ALA | A | 317 | 37.878 | 36.136 | 29.487 | 1.00 | 29.26 | C |
| ATOM | 2437 | C   | ALA | A | 317 | 38.776 | 36.941 | 30.389 | 1.00 | 28.08 | C |
| ATOM | 2438 | O   | ALA | A | 317 | 39.052 | 36.564 | 31.519 | 1.00 | 27.65 | O |
| ATOM | 2439 | CB  | ALA | A | 317 | 38.733 | 35.267 | 28.561 | 1.00 | 28.70 | C |
| ATOM | 2440 | N   | ILE | A | 318 | 39.211 | 38.068 | 29.873 | 1.00 | 28.33 | N |
| ATOM | 2441 | CA  | ILE | A | 318 | 40.083 | 38.945 | 30.628 | 1.00 | 28.40 | C |
| ATOM | 2442 | C   | ILE | A | 318 | 39.338 | 39.526 | 31.825 | 1.00 | 28.94 | C |
| ATOM | 2443 | O   | ILE | A | 318 | 39.880 | 39.503 | 32.924 | 1.00 | 29.70 | O |
| ATOM | 2444 | CB  | ILE | A | 318 | 40.697 | 40.053 | 29.732 | 1.00 | 27.74 | C |
| ATOM | 2445 | CG1 | ILE | A | 318 | 41.683 | 39.443 | 28.743 | 1.00 | 28.14 | C |
| ATOM | 2446 | CG2 | ILE | A | 318 | 41.433 | 41.082 | 30.577 | 1.00 | 27.98 | C |
| ATOM | 2447 | CD1 | ILE | A | 318 | 42.271 | 40.447 | 27.759 | 1.00 | 29.17 | C |
| ATOM | 2448 | N   | MET | A | 319 | 38.115 | 40.032 | 31.630 | 1.00 | 28.75 | N |
| ATOM | 2449 | CA  | MET | A | 319 | 37.402 | 40.666 | 32.735 | 1.00 | 28.64 | C |
| ATOM | 2450 | C   | MET | A | 319 | 37.140 | 39.669 | 33.877 | 1.00 | 29.22 | C |
| ATOM | 2451 | O   | MET | A | 319 | 37.308 | 39.981 | 35.082 | 1.00 | 30.32 | O |
| ATOM | 2452 | CB  | MET | A | 319 | 36.123 | 41.355 | 32.273 | 1.00 | 28.33 | C |
| ATOM | 2453 | CG  | MET | A | 319 | 36.327 | 42.553 | 31.334 | 1.00 | 27.88 | C |
| ATOM | 2454 | SD  | MET | A | 319 | 34.779 | 43.349 | 30.857 | 1.00 | 29.90 | S |
| ATOM | 2455 | CE  | MET | A | 319 | 34.146 | 42.288 | 29.455 | 1.00 | 28.71 | C |
| ATOM | 2456 | N   | ARG | A | 320 | 36.802 | 38.446 | 33.515 | 1.00 | 29.22 | N |
| ATOM | 2457 | CA  | ARG | A | 320 | 36.543 | 37.429 | 34.520 | 1.00 | 28.75 | C |
| ATOM | 2458 | C   | ARG | A | 320 | 37.806 | 37.221 | 35.325 | 1.00 | 28.81 | C |
| ATOM | 2459 | O   | ARG | A | 320 | 37.782 | 37.132 | 36.569 | 1.00 | 28.76 | O |
| ATOM | 2460 | CB  | ARG | A | 320 | 36.142 | 36.118 | 33.861 | 1.00 | 28.67 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2461 | CG  | ARG | A | 320 | 34.810 | 36.125 | 33.120 | 1.00 | 29.62 | C |
| ATOM | 2462 | CD  | ARG | A | 320 | 34.371 | 34.747 | 32.603 | 1.00 | 27.74 | C |
| ATOM | 2463 | NE  | ARG | A | 320 | 34.193 | 33.843 | 33.716 | 1.00 | 24.81 | N |
| ATOM | 2464 | CZ  | ARG | A | 320 | 33.161 | 33.887 | 34.526 | 1.00 | 27.65 | C |
| ATOM | 2465 | NH1 | ARG | A | 320 | 32.180 | 34.752 | 34.330 | 1.00 | 29.97 | N |
| ATOM | 2466 | NH2 | ARG | A | 320 | 33.088 | 33.064 | 35.542 | 1.00 | 27.59 | N |
| ATOM | 2467 | N   | ASN | A | 321 | 38.933 | 37.167 | 34.627 | 1.00 | 28.60 | N |
| ATOM | 2468 | CA  | ASN | A | 321 | 40.185 | 36.884 | 35.320 | 1.00 | 28.16 | C |
| ATOM | 2469 | C   | ASN | A | 321 | 40.526 | 38.003 | 36.291 | 1.00 | 28.13 | C |
| ATOM | 2470 | O   | ASN | A | 321 | 40.945 | 37.742 | 37.423 | 1.00 | 29.13 | O |
| ATOM | 2471 | CB  | ASN | A | 321 | 41.318 | 36.615 | 34.319 | 1.00 | 28.09 | C |
| ATOM | 2472 | CG  | ASN | A | 321 | 41.317 | 35.177 | 33.817 | 1.00 | 27.94 | C |
| ATOM | 2473 | OD1 | ASN | A | 321 | 40.924 | 34.286 | 34.555 | 1.00 | 28.53 | O |
| ATOM | 2474 | ND2 | ASN | A | 321 | 41.751 | 34.946 | 32.560 | 1.00 | 23.58 | N |
| ATOM | 2475 | N   | ILE | A | 322 | 40.337 | 39.250 | 35.876 | 1.00 | 27.49 | N |
| ATOM | 2476 | CA  | ILE | A | 322 | 40.659 | 40.350 | 36.749 | 1.00 | 27.70 | C |
| ATOM | 2477 | C   | ILE | A | 322 | 39.792 | 40.209 | 38.017 | 1.00 | 27.39 | C |
| ATOM | 2478 | O   | ILE | A | 322 | 40.284 | 40.315 | 39.101 | 1.00 | 26.48 | O |
| ATOM | 2479 | CB  | ILE | A | 322 | 40.353 | 41.680 | 36.059 | 1.00 | 28.04 | C |
| ATOM | 2480 | CG1 | ILE | A | 322 | 41.302 | 41.941 | 34.897 | 1.00 | 30.79 | C |
| ATOM | 2481 | CG2 | ILE | A | 322 | 40.426 | 42.832 | 37.038 | 1.00 | 28.09 | C |
| ATOM | 2482 | CD1 | ILE | A | 322 | 42.756 | 41.766 | 35.226 | 1.00 | 32.31 | C |
| ATOM | 2483 | N   | GLU | A | 323 | 38.494 | 39.961 | 37.854 | 1.00 | 27.37 | N |
| ATOM | 2484 | CA  | GLU | A | 323 | 37.618 | 39.868 | 38.985 | 1.00 | 27.48 | C |
| ATOM | 2485 | C   | GLU | A | 323 | 38.060 | 38.784 | 39.881 | 1.00 | 27.52 | C |
| ATOM | 2486 | O   | GLU | A | 323 | 38.096 | 38.956 | 41.079 | 1.00 | 26.90 | O |
| ATOM | 2487 | CB  | GLU | A | 323 | 36.183 | 39.637 | 38.558 | 1.00 | 27.48 | C |
| ATOM | 2488 | CG  | GLU | A | 323 | 35.592 | 40.849 | 37.910 | 1.00 | 27.65 | C |
| ATOM | 2489 | CD  | GLU | A | 323 | 34.199 | 40.631 | 37.318 | 1.00 | 25.69 | C |
| ATOM | 2490 | OE1 | GLU | A | 323 | 33.236 | 40.358 | 38.050 | 1.00 | 24.42 | O |
| ATOM | 2491 | OE2 | GLU | A | 323 | 34.072 | 40.808 | 36.101 | 1.00 | 24.98 | O |
| ATOM | 2492 | N   | LYS | A | 324 | 38.419 | 37.659 | 39.297 | 1.00 | 29.13 | N |
| ATOM | 2493 | CA  | LYS | A | 324 | 38.845 | 36.508 | 40.097 | 1.00 | 30.35 | C |
| ATOM | 2494 | C   | LYS | A | 324 | 40.099 | 36.825 | 40.912 | 1.00 | 31.16 | C |
| ATOM | 2495 | O   | LYS | A | 324 | 40.123 | 36.547 | 42.111 | 1.00 | 32.01 | O |
| ATOM | 2496 | CB  | LYS | A | 324 | 39.116 | 35.289 | 39.222 | 1.00 | 30.16 | C |
| ATOM | 2497 | CG  | LYS | A | 324 | 37.887 | 34.625 | 38.648 | 1.00 | 30.63 | C |
| ATOM | 2498 | CD  | LYS | A | 324 | 38.344 | 33.454 | 37.765 | 1.00 | 30.70 | C |
| ATOM | 2499 | CE  | LYS | A | 324 | 37.204 | 32.713 | 37.038 | 1.00 | 30.66 | C |
| ATOM | 2500 | NZ  | LYS | A | 324 | 37.728 | 31.451 | 36.325 | 1.00 | 27.19 | N |
| ATOM | 2501 | N   | MET | A | 325 | 41.119 | 37.401 | 40.270 | 1.00 | 31.84 | N |
| ATOM | 2502 | CA  | MET | A | 325 | 42.392 | 37.735 | 40.939 | 1.00 | 32.71 | C |
| ATOM | 2503 | C   | MET | A | 325 | 42.216 | 38.743 | 42.078 | 1.00 | 32.44 | C |
| ATOM | 2504 | O   | MET | A | 325 | 42.840 | 38.637 | 43.141 | 1.00 | 30.36 | O |
| ATOM | 2505 | CB  | MET | A | 325 | 43.417 | 38.276 | 39.923 | 1.00 | 32.98 | C |
| ATOM | 2506 | CG  | MET | A | 325 | 43.978 | 37.216 | 39.032 | 1.00 | 36.70 | C |
| ATOM | 2507 | SD  | MET | A | 325 | 44.734 | 37.879 | 37.532 | 1.00 | 46.02 | S |
| ATOM | 2508 | CE  | MET | A | 325 | 45.616 | 39.197 | 38.250 | 1.00 | 46.11 | C |
| ATOM | 2509 | N   | LEU | A | 326 | 41.376 | 39.738 | 41.837 | 1.00 | 33.01 | N |
| ATOM | 2510 | CA  | LEU | A | 326 | 41.116 | 40.756 | 42.852 | 1.00 | 34.17 | C |
| ATOM | 2511 | C   | LEU | A | 326 | 40.490 | 40.151 | 44.083 | 1.00 | 33.83 | C |
| ATOM | 2512 | O   | LEU | A | 326 | 40.871 | 40.464 | 45.188 | 1.00 | 33.22 | O |
| ATOM | 2513 | CB  | LEU | A | 326 | 40.185 | 41.818 | 42.305 | 1.00 | 34.61 | C |
| ATOM | 2514 | CG  | LEU | A | 326 | 40.740 | 43.194 | 41.974 | 1.00 | 37.32 | C |
| ATOM | 2515 | CD1 | LEU | A | 326 | 42.251 | 43.297 | 41.924 | 1.00 | 39.32 | C |
| ATOM | 2516 | CD2 | LEU | A | 326 | 40.158 | 43.607 | 40.643 | 1.00 | 39.20 | C |
| ATOM | 2517 | N   | GLY | A | 327 | 39.534 | 39.262 | 43.861 | 1.00 | 34.50 | N |
| ATOM | 2518 | CA  | GLY | A | 327 | 38.842 | 38.569 | 44.930 | 1.00 | 34.87 | C |
| ATOM | 2519 | C   | GLY | A | 327 | 39.796 | 37.776 | 45.779 | 1.00 | 35.34 | C |
| ATOM | 2520 | O   | GLY | A | 327 | 39.728 | 37.810 | 47.016 | 1.00 | 35.51 | O |
| ATOM | 2521 | N   | GLU | A | 328 | 40.725 | 37.081 | 45.139 | 1.00 | 35.88 | N |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2522 | CA  | GLU | A | 328 | 41.708 | 36.346 | 45.926 | 1.00 | 36.96 | C |
| ATOM | 2523 | C   | GLU | A | 328 | 42.668 | 37.302 | 46.614 | 1.00 | 35.46 | C |
| ATOM | 2524 | O   | GLU | A | 328 | 42.958 | 37.144 | 47.799 | 1.00 | 35.65 | O |
| ATOM | 2525 | CB  | GLU | A | 328 | 42.465 | 35.340 | 45.074 | 1.00 | 37.89 | C |
| ATOM | 2526 | CG  | GLU | A | 328 | 41.555 | 34.272 | 44.481 | 1.00 | 43.40 | C |
| ATOM | 2527 | CD  | GLU | A | 328 | 41.694 | 32.905 | 45.135 | 1.00 | 50.39 | C |
| ATOM | 2528 | OE1 | GLU | A | 328 | 42.006 | 32.861 | 46.361 | 1.00 | 53.07 | O |
| ATOM | 2529 | OE2 | GLU | A | 328 | 41.503 | 31.876 | 44.396 | 1.00 | 53.24 | O |
| ATOM | 2530 | N   | ALA | A | 329 | 43.110 | 38.331 | 45.906 | 1.00 | 34.23 | N |
| ATOM | 2531 | CA  | ALA | A | 329 | 44.130 | 39.208 | 46.469 | 1.00 | 33.82 | C |
| ATOM | 2532 | C   | ALA | A | 329 | 43.652 | 40.031 | 47.632 | 1.00 | 33.70 | C |
| ATOM | 2533 | O   | ALA | A | 329 | 44.384 | 40.279 | 48.547 | 1.00 | 33.79 | O |
| ATOM | 2534 | CB  | ALA | A | 329 | 44.711 | 40.079 | 45.428 | 1.00 | 33.36 | C |
| ATOM | 2535 | N   | LEU | A | 330 | 42.410 | 40.451 | 47.602 | 1.00 | 34.57 | N |
| ATOM | 2536 | CA  | LEU | A | 330 | 41.869 | 41.243 | 48.694 | 1.00 | 35.04 | C |
| ATOM | 2537 | C   | LEU | A | 330 | 41.351 | 40.397 | 49.837 | 1.00 | 35.29 | C |
| ATOM | 2538 | O   | LEU | A | 330 | 41.011 | 40.922 | 50.884 | 1.00 | 35.39 | O |
| ATOM | 2539 | CB  | LEU | A | 330 | 40.721 | 42.096 | 48.182 | 1.00 | 34.85 | C |
| ATOM | 2540 | CG  | LEU | A | 330 | 41.141 | 43.081 | 47.095 | 1.00 | 35.83 | C |
| ATOM | 2541 | CD1 | LEU | A | 330 | 39.907 | 43.564 | 46.304 | 1.00 | 37.05 | C |
| ATOM | 2542 | CD2 | LEU | A | 330 | 41.842 | 44.244 | 47.662 | 1.00 | 34.12 | C |
| ATOM | 2543 | N   | GLY | A | 331 | 41.223 | 39.098 | 49.619 | 1.00 | 36.20 | N |
| ATOM | 2544 | CA  | GLY | A | 331 | 40.751 | 38.207 | 50.659 | 1.00 | 36.87 | C |
| ATOM | 2545 | C   | GLY | A | 331 | 39.260 | 38.250 | 50.957 | 1.00 | 37.48 | C |
| ATOM | 2546 | O   | GLY | A | 331 | 38.807 | 37.527 | 51.846 | 1.00 | 38.53 | O |
| ATOM | 2547 | N   | ASN | A | 332 | 38.509 | 39.085 | 50.242 | 1.00 | 37.67 | N |
| ATOM | 2548 | CA  | ASN | A | 332 | 37.069 | 39.175 | 50.399 | 1.00 | 38.06 | C |
| ATOM | 2549 | C   | ASN | A | 332 | 36.446 | 39.652 | 49.088 | 1.00 | 37.75 | C |
| ATOM | 2550 | O   | ASN | A | 332 | 36.688 | 40.760 | 48.661 | 1.00 | 37.42 | O |
| ATOM | 2551 | CB  | ASN | A | 332 | 36.728 | 40.152 | 51.523 | 1.00 | 38.50 | C |
| ATOM | 2552 | CG  | ASN | A | 332 | 35.272 | 40.103 | 51.896 | 1.00 | 40.34 | C |
| ATOM | 2553 | OD1 | ASN | A | 332 | 34.493 | 39.377 | 51.274 | 1.00 | 43.85 | O |
| ATOM | 2554 | ND2 | ASN | A | 332 | 34.894 | 40.841 | 52.937 | 1.00 | 41.75 | N |
| ATOM | 2555 | N   | PRO | A | 333 | 35.628 | 38.839 | 48.451 | 1.00 | 37.92 | N |
| ATOM | 2556 | CA  | PRO | A | 333 | 35.076 | 39.209 | 47.146 | 1.00 | 37.97 | C |
| ATOM | 2557 | C   | PRO | A | 333 | 34.245 | 40.456 | 47.211 | 1.00 | 37.96 | C |
| ATOM | 2558 | O   | PRO | A | 333 | 34.086 | 41.143 | 46.204 | 1.00 | 37.81 | O |
| ATOM | 2559 | CB  | PRO | A | 333 | 34.182 | 38.024 | 46.770 | 1.00 | 37.85 | C |
| ATOM | 2560 | CG  | PRO | A | 333 | 34.327 | 37.037 | 47.801 | 1.00 | 38.26 | C |
| ATOM | 2561 | CD  | PRO | A | 333 | 35.161 | 37.530 | 48.908 | 1.00 | 37.98 | C |
| ATOM | 2562 | N   | GLN | A | 334 | 33.702 | 40.741 | 48.381 | 1.00 | 38.23 | N |
| ATOM | 2563 | CA  | GLN | A | 334 | 32.872 | 41.928 | 48.539 | 1.00 | 38.84 | C |
| ATOM | 2564 | C   | GLN | A | 334 | 33.713 | 43.177 | 48.442 | 1.00 | 37.04 | C |
| ATOM | 2565 | O   | GLN | A | 334 | 33.185 | 44.254 | 48.276 | 1.00 | 37.42 | O |
| ATOM | 2566 | CB  | GLN | A | 334 | 32.041 | 41.870 | 49.850 | 1.00 | 39.97 | C |
| ATOM | 2567 | CG  | GLN | A | 334 | 30.696 | 41.057 | 49.612 | 1.00 | 44.72 | C |
| ATOM | 2568 | CD  | GLN | A | 334 | 29.669 | 41.117 | 50.756 | 1.00 | 49.62 | C |
| ATOM | 2569 | OE1 | GLN | A | 334 | 29.666 | 42.067 | 51.566 | 1.00 | 53.65 | O |
| ATOM | 2570 | NE2 | GLN | A | 334 | 28.781 | 40.106 | 50.808 | 1.00 | 50.33 | N |
| ATOM | 2571 | N   | GLU | A | 335 | 35.026 | 43.036 | 48.489 | 1.00 | 35.15 | N |
| ATOM | 2572 | CA  | GLU | A | 335 | 35.872 | 44.193 | 48.385 | 1.00 | 34.55 | C |
| ATOM | 2573 | C   | GLU | A | 335 | 36.197 | 44.510 | 46.927 | 1.00 | 33.05 | C |
| ATOM | 2574 | O   | GLU | A | 335 | 36.760 | 45.564 | 46.640 | 1.00 | 32.79 | O |
| ATOM | 2575 | CB  | GLU | A | 335 | 37.144 | 44.028 | 49.247 | 1.00 | 35.19 | C |
| ATOM | 2576 | CG  | GLU | A | 335 | 36.927 | 44.326 | 50.727 | 1.00 | 37.92 | C |
| ATOM | 2577 | CD  | GLU | A | 335 | 38.195 | 44.232 | 51.550 | 1.00 | 43.46 | C |
| ATOM | 2578 | OE1 | GLU | A | 335 | 39.179 | 44.916 | 51.179 | 1.00 | 46.92 | O |
| ATOM | 2579 | OE2 | GLU | A | 335 | 38.211 | 43.499 | 52.589 | 1.00 | 49.17 | O |
| ATOM | 2580 | N   | VAL | A | 336 | 35.792 | 43.633 | 46.005 | 1.00 | 31.25 | N |
| ATOM | 2581 | CA  | VAL | A | 336 | 36.081 | 43.810 | 44.579 | 1.00 | 29.91 | C |
| ATOM | 2582 | C   | VAL | A | 336 | 35.505 | 45.076 | 43.957 | 1.00 | 29.08 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2583 | O   | VAL | A | 336 | 36.177 | 45.816 | 43.246 | 1.00 | 29.08 | O |
| ATOM | 2584 | CB  | VAL | A | 336 | 35.648 | 42.584 | 43.791 | 1.00 | 30.21 | C |
| ATOM | 2585 | CG1 | VAL | A | 336 | 35.743 | 42.805 | 42.325 | 1.00 | 29.11 | C |
| ATOM | 2586 | CG2 | VAL | A | 336 | 36.540 | 41.391 | 44.161 | 1.00 | 29.98 | C |
| ATOM | 2587 | N   | GLY | A | 337 | 34.263 | 45.354 | 44.240 | 1.00 | 28.54 | N |
| ATOM | 2588 | CA  | GLY | A | 337 | 33.644 | 46.546 | 43.722 | 1.00 | 27.74 | C |
| ATOM | 2589 | C   | GLY | A | 337 | 34.285 | 47.848 | 44.130 | 1.00 | 27.24 | C |
| ATOM | 2590 | O   | GLY | A | 337 | 34.599 | 48.687 | 43.281 | 1.00 | 26.81 | O |
| ATOM | 2591 | N   | PRO | A | 338 | 34.365 | 48.094 | 45.428 | 1.00 | 27.19 | N |
| ATOM | 2592 | CA  | PRO | A | 338 | 34.994 | 49.334 | 45.905 | 1.00 | 26.74 | C |
| ATOM | 2593 | C   | PRO | A | 338 | 36.378 | 49.553 | 45.328 | 1.00 | 26.42 | C |
| ATOM | 2594 | O   | PRO | A | 338 | 36.678 | 50.668 | 44.932 | 1.00 | 27.57 | O |
| ATOM | 2595 | CB  | PRO | A | 338 | 35.008 | 49.173 | 47.426 | 1.00 | 25.92 | C |
| ATOM | 2596 | CG  | PRO | A | 338 | 33.800 | 48.384 | 47.682 | 1.00 | 27.15 | C |
| ATOM | 2597 | CD  | PRO | A | 338 | 33.750 | 47.326 | 46.531 | 1.00 | 27.09 | C |
| ATOM | 2598 | N   | LEU | A | 339 | 37.199 | 48.533 | 45.225 | 1.00 | 25.95 | N |
| ATOM | 2599 | CA  | LEU | A | 339 | 38.505 | 48.762 | 44.652 | 1.00 | 26.15 | C |
| ATOM | 2600 | C   | LEU | A | 339 | 38.384 | 49.205 | 43.192 | 1.00 | 25.74 | C |
| ATOM | 2601 | O   | LEU | A | 339 | 39.021 | 50.203 | 42.784 | 1.00 | 23.97 | O |
| ATOM | 2602 | CB  | LEU | A | 339 | 39.375 | 47.521 | 44.763 | 1.00 | 27.19 | C |
| ATOM | 2603 | CG  | LEU | A | 339 | 40.835 | 47.787 | 44.367 | 1.00 | 28.71 | C |
| ATOM | 2604 | CD1 | LEU | A | 339 | 41.805 | 47.124 | 45.241 | 1.00 | 31.14 | C |
| ATOM | 2605 | CD2 | LEU | A | 339 | 41.028 | 47.264 | 42.987 | 1.00 | 30.12 | C |
| ATOM | 2606 | N   | LEU | A | 340 | 37.555 | 48.491 | 42.416 | 1.00 | 25.64 | N |
| ATOM | 2607 | CA  | LEU | A | 340 | 37.364 | 48.841 | 40.991 | 1.00 | 25.90 | C |
| ATOM | 2608 | C   | LEU | A | 340 | 36.860 | 50.261 | 40.871 | 1.00 | 26.04 | C |
| ATOM | 2609 | O   | LEU | A | 340 | 37.324 | 51.044 | 40.034 | 1.00 | 25.93 | O |
| ATOM | 2610 | CB  | LEU | A | 340 | 36.399 | 47.900 | 40.293 | 1.00 | 25.64 | C |
| ATOM | 2611 | CG  | LEU | A | 340 | 36.996 | 46.521 | 40.072 | 1.00 | 27.50 | C |
| ATOM | 2612 | CD1 | LEU | A | 340 | 35.943 | 45.559 | 39.555 | 1.00 | 26.88 | C |
| ATOM | 2613 | CD2 | LEU | A | 340 | 38.221 | 46.587 | 39.138 | 1.00 | 26.63 | C |
| ATOM | 2614 | N   | ASN | A | 341 | 35.914 | 50.610 | 41.720 | 1.00 | 26.45 | N |
| ATOM | 2615 | CA  | ASN | A | 341 | 35.377 | 51.963 | 41.669 | 1.00 | 27.35 | C |
| ATOM | 2616 | C   | ASN | A | 341 | 36.450 | 52.983 | 41.983 | 1.00 | 27.08 | C |
| ATOM | 2617 | O   | ASN | A | 341 | 36.578 | 54.012 | 41.324 | 1.00 | 26.82 | O |
| ATOM | 2618 | CB  | ASN | A | 341 | 34.183 | 52.117 | 42.619 | 1.00 | 27.50 | C |
| ATOM | 2619 | CG  | ASN | A | 341 | 32.901 | 51.709 | 41.975 | 1.00 | 28.85 | C |
| ATOM | 2620 | OD1 | ASN | A | 341 | 32.509 | 52.283 | 40.957 | 1.00 | 37.23 | O |
| ATOM | 2621 | ND2 | ASN | A | 341 | 32.263 | 50.697 | 42.504 | 1.00 | 29.29 | N |
| ATOM | 2622 | N   | THR | A | 342 | 37.234 | 52.665 | 42.994 | 1.00 | 26.89 | N |
| ATOM | 2623 | CA  | THR | A | 342 | 38.321 | 53.509 | 43.355 | 1.00 | 27.22 | C |
| ATOM | 2624 | C   | THR | A | 342 | 39.301 | 53.629 | 42.191 | 1.00 | 27.16 | C |
| ATOM | 2625 | O   | THR | A | 342 | 39.861 | 54.686 | 42.003 | 1.00 | 26.86 | O |
| ATOM | 2626 | CB  | THR | A | 342 | 38.995 | 52.934 | 44.568 | 1.00 | 27.76 | C |
| ATOM | 2627 | OG1 | THR | A | 342 | 38.212 | 53.248 | 45.734 | 1.00 | 29.14 | O |
| ATOM | 2628 | CG2 | THR | A | 342 | 40.367 | 53.604 | 44.784 | 1.00 | 28.62 | C |
| ATOM | 2629 | N   | MET | A | 343 | 39.502 | 52.560 | 41.419 | 1.00 | 26.80 | N |
| ATOM | 2630 | CA  | MET | A | 343 | 40.401 | 52.623 | 40.282 | 1.00 | 27.48 | C |
| ATOM | 2631 | C   | MET | A | 343 | 39.927 | 53.552 | 39.174 | 1.00 | 27.78 | C |
| ATOM | 2632 | O   | MET | A | 343 | 40.762 | 54.229 | 38.554 | 1.00 | 26.44 | O |
| ATOM | 2633 | CB  | MET | A | 343 | 40.602 | 51.253 | 39.634 | 1.00 | 28.13 | C |
| ATOM | 2634 | CG  | MET | A | 343 | 41.758 | 50.440 | 40.125 | 1.00 | 30.19 | C |
| ATOM | 2635 | SD  | MET | A | 343 | 42.279 | 49.088 | 38.964 | 1.00 | 32.27 | S |
| ATOM | 2636 | CE  | MET | A | 343 | 41.049 | 48.127 | 39.221 | 1.00 | 34.83 | C |
| ATOM | 2637 | N   | ILE | A | 344 | 38.619 | 53.568 | 38.864 | 1.00 | 28.41 | N |
| ATOM | 2638 | CA  | ILE | A | 344 | 38.193 | 54.350 | 37.700 | 1.00 | 29.03 | C |
| ATOM | 2639 | C   | ILE | A | 344 | 37.712 | 55.748 | 37.957 | 1.00 | 28.17 | C |
| ATOM | 2640 | O   | ILE | A | 344 | 37.879 | 56.587 | 37.064 | 1.00 | 27.26 | O |
| ATOM | 2641 | CB  | ILE | A | 344 | 37.146 | 53.650 | 36.818 | 1.00 | 29.47 | C |
| ATOM | 2642 | CG1 | ILE | A | 344 | 35.766 | 53.866 | 37.384 | 1.00 | 32.69 | C |
| ATOM | 2643 | CG2 | ILE | A | 344 | 37.457 | 52.176 | 36.667 | 1.00 | 32.43 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2644 | CD1 | ILE | A | 344 | 34.724 | 53.358 | 36.590 | 1.00 | 35.46 | C |
| ATOM | 2645 | N   | LYS | A | 345 | 37.107 | 56.032 | 39.108 | 1.00 | 27.79 | N |
| ATOM | 2646 | CA  | LYS | A | 345 | 36.518 | 57.364 | 39.218 | 1.00 | 28.48 | C |
| ATOM | 2647 | C   | LYS | A | 345 | 37.489 | 58.485 | 39.219 | 1.00 | 27.72 | C |
| ATOM | 2648 | O   | LYS | A | 345 | 38.428 | 58.555 | 40.000 | 1.00 | 27.37 | O |
| ATOM | 2649 | CB  | LYS | A | 345 | 35.542 | 57.611 | 40.343 | 1.00 | 29.78 | C |
| ATOM | 2650 | CG  | LYS | A | 345 | 35.537 | 56.758 | 41.491 | 1.00 | 34.49 | C |
| ATOM | 2651 | CD  | LYS | A | 345 | 34.075 | 56.352 | 41.692 | 1.00 | 37.43 | C |
| ATOM | 2652 | CE  | LYS | A | 345 | 33.508 | 57.036 | 42.904 | 1.00 | 40.47 | C |
| ATOM | 2653 | NZ  | LYS | A | 345 | 34.223 | 56.522 | 44.138 | 1.00 | 46.19 | N |
| ATOM | 2654 | N   | GLY | A | 346 | 37.218 | 59.386 | 38.297 | 1.00 | 26.82 | N |
| ATOM | 2655 | CA  | GLY | A | 346 | 38.044 | 60.538 | 38.108 | 1.00 | 25.95 | C |
| ATOM | 2656 | C   | GLY | A | 346 | 39.314 | 60.175 | 37.392 | 1.00 | 25.08 | C |
| ATOM | 2657 | O   | GLY | A | 346 | 40.172 | 61.022 | 37.244 | 1.00 | 24.91 | O |
| ATOM | 2658 | N   | ARG | A | 347 | 39.419 | 58.935 | 36.944 | 1.00 | 24.84 | N |
| ATOM | 2659 | CA  | ARG | A | 347 | 40.647 | 58.436 | 36.347 | 1.00 | 25.30 | C |
| ATOM | 2660 | C   | ARG | A | 347 | 40.431 | 57.848 | 34.937 | 1.00 | 26.05 | C |
| ATOM | 2661 | O   | ARG | A | 347 | 41.138 | 58.196 | 34.007 | 1.00 | 24.59 | O |
| ATOM | 2662 | CB  | ARG | A | 347 | 41.279 | 57.395 | 37.272 | 1.00 | 25.27 | C |
| ATOM | 2663 | CG  | ARG | A | 347 | 41.716 | 57.934 | 38.696 | 1.00 | 24.21 | C |
| ATOM | 2664 | CD  | ARG | A | 347 | 43.159 | 57.506 | 39.082 | 1.00 | 25.10 | C |
| ATOM | 2665 | NE  | ARG | A | 347 | 43.175 | 56.084 | 39.017 | 1.00 | 24.49 | N |
| ATOM | 2666 | CZ  | ARG | A | 347 | 44.102 | 55.293 | 38.566 | 1.00 | 19.51 | C |
| ATOM | 2667 | NH1 | ARG | A | 347 | 45.299 | 55.692 | 38.195 | 1.00 | 21.86 | N |
| ATOM | 2668 | NH2 | ARG | A | 347 | 43.802 | 54.011 | 38.579 | 1.00 | 18.94 | N |
| ATOM | 2669 | N   | TYR | A | 348 | 39.438 | 56.991 | 34.794 | 1.00 | 27.91 | N |
| ATOM | 2670 | CA  | TYR | A | 348 | 39.119 | 56.380 | 33.507 | 1.00 | 29.80 | C |
| ATOM | 2671 | C   | TYR | A | 348 | 37.671 | 56.590 | 33.065 | 1.00 | 32.00 | C |
| ATOM | 2672 | O   | TYR | A | 348 | 37.309 | 56.173 | 31.964 | 1.00 | 32.29 | O |
| ATOM | 2673 | CB  | TYR | A | 348 | 39.379 | 54.877 | 33.543 | 1.00 | 28.38 | C |
| ATOM | 2674 | CG  | TYR | A | 348 | 40.836 | 54.498 | 33.597 | 1.00 | 27.86 | C |
| ATOM | 2675 | CD1 | TYR | A | 348 | 41.617 | 54.473 | 32.446 | 1.00 | 26.79 | C |
| ATOM | 2676 | CD2 | TYR | A | 348 | 41.422 | 54.124 | 34.787 | 1.00 | 25.32 | C |
| ATOM | 2677 | CE1 | TYR | A | 348 | 42.945 | 54.106 | 32.496 | 1.00 | 25.35 | C |
| ATOM | 2678 | CE2 | TYR | A | 348 | 42.734 | 53.762 | 34.847 | 1.00 | 27.07 | C |
| ATOM | 2679 | CZ  | TYR | A | 348 | 43.507 | 53.759 | 33.700 | 1.00 | 26.40 | C |
| ATOM | 2680 | OH  | TYR | A | 348 | 44.827 | 53.378 | 33.789 | 1.00 | 22.93 | O |
| ATOM | 2681 | N   | ASN | A | 349 | 36.824 | 57.193 | 33.894 | 1.00 | 34.78 | N |
| ATOM | 2682 | CA  | ASN | A | 349 | 35.426 | 57.360 | 33.473 | 1.00 | 37.16 | C |
| ATOM | 2683 | C   | ASN | A | 349 | 34.997 | 58.760 | 33.104 | 1.00 | 38.90 | C |
| ATOM | 2684 | O   | ASN | A | 349 | 35.690 | 59.756 | 33.136 | 1.00 | 38.66 | O |
| ATOM | 2685 | CB  | ASN | A | 349 | 34.474 | 56.837 | 34.493 | 1.00 | 36.69 | C |
| ATOM | 2686 | CG  | ASN | A | 349 | 34.480 | 57.633 | 35.727 | 1.00 | 39.34 | C |
| ATOM | 2687 | OD1 | ASN | A | 349 | 35.229 | 58.632 | 35.875 | 1.00 | 40.92 | O |
| ATOM | 2688 | ND2 | ASN | A | 349 | 33.654 | 57.188 | 36.684 | 1.00 | 42.73 | N |
| ATOM | 2689 | OXT | ASN | A | 349 | 33.854 | 58.954 | 32.689 | 1.00 | 44.16 | O |
| TER  | 2690 |     | ASN | A | 349 |        |        |        |      |       |   |
| ATOM | 2691 | N   | LEU | S | 795 | 45.870 | 35.442 | 31.163 | 1.00 | 49.68 | N |
| ATOM | 2692 | CA  | LEU | S | 795 | 44.790 | 36.472 | 31.262 | 1.00 | 49.90 | C |
| ATOM | 2693 | C   | LEU | S | 795 | 43.668 | 36.155 | 30.294 | 1.00 | 50.12 | C |
| ATOM | 2694 | O   | LEU | S | 795 | 42.492 | 36.182 | 30.666 | 1.00 | 49.41 | O |
| ATOM | 2695 | CB  | LEU | S | 795 | 45.331 | 37.873 | 31.004 | 1.00 | 50.09 | C |
| ATOM | 2696 | CG  | LEU | S | 795 | 44.774 | 38.924 | 31.976 | 1.00 | 50.19 | C |
| ATOM | 2697 | CD1 | LEU | S | 795 | 44.929 | 38.464 | 33.388 | 1.00 | 50.50 | C |
| ATOM | 2698 | CD2 | LEU | S | 795 | 45.436 | 40.280 | 31.876 | 1.00 | 51.23 | C |
| ATOM | 2699 | N   | THR | S | 796 | 44.041 | 35.979 | 29.033 | 1.00 | 50.69 | N |
| ATOM | 2700 | CA  | THR | S | 796 | 43.178 | 35.421 | 27.997 | 1.00 | 51.67 | C |
| ATOM | 2701 | C   | THR | S | 796 | 42.734 | 33.983 | 28.241 | 1.00 | 51.11 | C |
| ATOM | 2702 | O   | THR | S | 796 | 41.884 | 33.464 | 27.535 | 1.00 | 51.41 | O |
| ATOM | 2703 | CB  | THR | S | 796 | 43.888 | 35.547 | 26.626 | 1.00 | 51.86 | C |
| ATOM | 2704 | OG1 | THR | S | 796 | 43.253 | 34.704 | 25.671 | 1.00 | 56.26 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2705 | CG2 | THR | S | 796 | 45.272 | 34.981 | 26.662 | 1.00 | 52.69 | C |
| ATOM | 2706 | N   | SER | S | 797 | 43.261 | 33.330 | 29.248 | 1.00 | 51.51 | N |
| ATOM | 2707 | CA  | SER | S | 797 | 42.838 | 31.965 | 29.497 | 1.00 | 52.74 | C |
| ATOM | 2708 | C   | SER | S | 797 | 41.471 | 31.865 | 30.165 | 1.00 | 53.39 | C |
| ATOM | 2709 | O   | SER | S | 797 | 41.070 | 32.733 | 30.934 | 1.00 | 52.91 | O |
| ATOM | 2710 | CB  | SER | S | 797 | 43.850 | 31.247 | 30.351 | 1.00 | 52.86 | C |
| ATOM | 2711 | OG  | SER | S | 797 | 43.687 | 31.623 | 31.697 | 1.00 | 55.21 | O |
| ATOM | 2712 | N   | TYR | S | 798 | 40.783 | 30.761 | 29.904 | 1.00 | 54.79 | N |
| ATOM | 2713 | CA  | TYR | S | 798 | 39.424 | 30.584 | 30.372 | 1.00 | 56.02 | C |
| ATOM | 2714 | C   | TYR | S | 798 | 39.168 | 29.271 | 31.042 | 1.00 | 55.81 | C |
| ATOM | 2715 | O   | TYR | S | 798 | 39.880 | 28.305 | 30.827 | 1.00 | 56.61 | O |
| ATOM | 2716 | CB  | TYR | S | 798 | 38.437 | 30.747 | 29.214 | 1.00 | 56.97 | C |
| ATOM | 2717 | CG  | TYR | S | 798 | 38.599 | 29.821 | 28.015 | 1.00 | 60.68 | C |
| ATOM | 2718 | CD1 | TYR | S | 798 | 39.595 | 30.035 | 27.059 | 1.00 | 62.78 | C |
| ATOM | 2719 | CD2 | TYR | S | 798 | 37.689 | 28.783 | 27.793 | 1.00 | 64.68 | C |
| ATOM | 2720 | CE1 | TYR | S | 798 | 39.708 | 29.207 | 25.943 | 1.00 | 65.08 | C |
| ATOM | 2721 | CE2 | TYR | S | 798 | 37.798 | 27.944 | 26.669 | 1.00 | 66.15 | C |
| ATOM | 2722 | CZ  | TYR | S | 798 | 38.808 | 28.155 | 25.755 | 1.00 | 65.29 | C |
| ATOM | 2723 | OH  | TYR | S | 798 | 38.902 | 27.335 | 24.652 | 1.00 | 64.08 | O |
| ATOM | 2724 | N   | ASP | S | 799 | 38.117 | 29.240 | 31.843 | 1.00 | 55.66 | N |
| ATOM | 2725 | CA  | ASP | S | 799 | 37.727 | 28.032 | 32.546 | 1.00 | 55.90 | C |
| ATOM | 2726 | C   | ASP | S | 799 | 36.636 | 27.385 | 31.739 | 1.00 | 54.64 | C |
| ATOM | 2727 | O   | ASP | S | 799 | 36.430 | 27.785 | 30.604 | 1.00 | 55.18 | O |
| ATOM | 2728 | CB  | ASP | S | 799 | 37.212 | 28.367 | 33.948 | 1.00 | 56.52 | C |
| ATOM | 2729 | CG  | ASP | S | 799 | 37.366 | 27.225 | 34.906 | 1.00 | 57.36 | C |
| ATOM | 2730 | OD1 | ASP | S | 799 | 36.749 | 26.147 | 34.720 | 1.00 | 57.64 | O |
| ATOM | 2731 | OD2 | ASP | S | 799 | 38.108 | 27.331 | 35.881 | 1.00 | 62.28 | O |
| ATOM | 2732 | N   | CYS | S | 800 | 35.915 | 26.428 | 32.326 | 1.00 | 53.45 | N |
| ATOM | 2733 | CA  | CYS | S | 800 | 34.887 | 25.693 | 31.594 | 1.00 | 52.63 | C |
| ATOM | 2734 | C   | CYS | S | 800 | 33.564 | 25.644 | 32.359 | 1.00 | 51.79 | C |
| ATOM | 2735 | O   | CYS | S | 800 | 32.871 | 24.632 | 32.357 | 1.00 | 51.30 | O |
| ATOM | 2736 | CB  | CYS | S | 800 | 35.372 | 24.282 | 31.327 | 1.00 | 52.47 | C |
| ATOM | 2737 | SG  | CYS | S | 800 | 35.703 | 23.408 | 32.872 | 1.00 | 52.72 | S |
| ATOM | 2738 | N   | GLU | S | 801 | 33.187 | 26.742 | 32.996 | 1.00 | 50.91 | N |
| ATOM | 2739 | CA  | GLU | S | 801 | 31.939 | 26.732 | 33.762 | 1.00 | 50.65 | C |
| ATOM | 2740 | C   | GLU | S | 801 | 30.657 | 26.939 | 32.909 | 1.00 | 50.18 | C |
| ATOM | 2741 | O   | GLU | S | 801 | 30.617 | 27.687 | 31.928 | 1.00 | 48.39 | O |
| ATOM | 2742 | CB  | GLU | S | 801 | 32.008 | 27.713 | 34.929 | 1.00 | 50.49 | C |
| ATOM | 2743 | CG  | GLU | S | 801 | 33.199 | 27.450 | 35.853 | 1.00 | 51.78 | C |
| ATOM | 2744 | CD  | GLU | S | 801 | 33.234 | 28.359 | 37.092 | 1.00 | 51.24 | C |
| ATOM | 2745 | OE1 | GLU | S | 801 | 32.589 | 28.038 | 38.102 | 1.00 | 49.25 | O |
| ATOM | 2746 | OE2 | GLU | S | 801 | 33.919 | 29.395 | 37.063 | 1.00 | 51.89 | O |
| ATOM | 2747 | N   | VAL | S | 802 | 29.624 | 26.213 | 33.320 | 1.00 | 50.54 | N |
| ATOM | 2748 | CA  | VAL | S | 802 | 28.338 | 26.161 | 32.650 | 1.00 | 50.71 | C |
| ATOM | 2749 | C   | VAL | S | 802 | 27.213 | 26.094 | 33.694 | 1.00 | 51.25 | C |
| ATOM | 2750 | O   | VAL | S | 802 | 27.464 | 25.960 | 34.885 | 1.00 | 50.69 | O |
| ATOM | 2751 | CB  | VAL | S | 802 | 28.286 | 24.902 | 31.746 | 1.00 | 50.61 | C |
| ATOM | 2752 | CG1 | VAL | S | 802 | 29.420 | 24.932 | 30.727 | 1.00 | 49.62 | C |
| ATOM | 2753 | CG2 | VAL | S | 802 | 28.376 | 23.601 | 32.585 | 1.00 | 49.78 | C |
| ATOM | 2754 | N   | ASN | S | 803 | 25.967 | 26.165 | 33.239 | 1.00 | 52.55 | N |
| ATOM | 2755 | CA  | ASN | S | 803 | 24.816 | 26.099 | 34.140 | 1.00 | 53.28 | C |
| ATOM | 2756 | C   | ASN | S | 803 | 24.516 | 24.663 | 34.561 | 1.00 | 54.95 | C |
| ATOM | 2757 | O   | ASN | S | 803 | 23.440 | 24.150 | 34.298 | 1.00 | 54.22 | O |
| ATOM | 2758 | CB  | ASN | S | 803 | 23.560 | 26.724 | 33.511 | 1.00 | 53.04 | C |
| ATOM | 2759 | CG  | ASN | S | 803 | 23.546 | 28.245 | 33.569 | 1.00 | 51.60 | C |
| ATOM | 2760 | OD1 | ASN | S | 803 | 24.576 | 28.895 | 33.755 | 1.00 | 51.13 | O |
| ATOM | 2761 | ND2 | ASN | S | 803 | 22.367 | 28.817 | 33.406 | 1.00 | 46.28 | N |
| ATOM | 2762 | N   | ALA | S | 804 | 25.498 | 24.033 | 35.201 | 1.00 | 57.29 | N |
| ATOM | 2763 | CA  | ALA | S | 804 | 25.373 | 22.697 | 35.784 | 1.00 | 59.38 | C |
| ATOM | 2764 | C   | ALA | S | 804 | 26.596 | 22.490 | 36.676 | 1.00 | 61.01 | C |
| ATOM | 2765 | O   | ALA | S | 804 | 27.667 | 23.026 | 36.407 | 1.00 | 61.45 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2766 | CB  | ALA | S | 804 | 25.315 | 21.603 | 34.716 | 1.00 | 59.47 | C |
| ATOM | 2767 | N   | PRO | S | 805 | 26.438 | 21.707 | 37.732 | 1.00 | 62.94 | N |
| ATOM | 2768 | CA  | PRO | S | 805 | 27.547 | 21.398 | 38.652 | 1.00 | 63.79 | C |
| ATOM | 2769 | C   | PRO | S | 805 | 28.616 | 20.498 | 38.003 | 1.00 | 64.48 | C |
| ATOM | 2770 | O   | PRO | S | 805 | 28.368 | 19.875 | 36.970 | 1.00 | 65.26 | O |
| ATOM | 2771 | CB  | PRO | S | 805 | 26.851 | 20.654 | 39.807 | 1.00 | 63.79 | C |
| ATOM | 2772 | CG  | PRO | S | 805 | 25.582 | 20.066 | 39.187 | 1.00 | 63.48 | C |
| ATOM | 2773 | CD  | PRO | S | 805 | 25.175 | 21.035 | 38.107 | 1.00 | 63.26 | C |
| ATOM | 2774 | N   | ILE | S | 806 | 29.779 | 20.405 | 38.630 | 1.00 | 65.18 | N |
| ATOM | 2775 | CA  | ILE | S | 806 | 30.903 | 19.626 | 38.100 | 1.00 | 65.66 | C |
| ATOM | 2776 | C   | ILE | S | 806 | 30.853 | 18.145 | 38.489 | 1.00 | 65.84 | C |
| ATOM | 2777 | O   | ILE | S | 806 | 30.287 | 17.780 | 39.522 | 1.00 | 66.22 | O |
| ATOM | 2778 | CB  | ILE | S | 806 | 32.239 | 20.255 | 38.582 | 1.00 | 65.91 | C |
| ATOM | 2779 | CG1 | ILE | S | 806 | 32.435 | 20.046 | 40.089 | 1.00 | 65.62 | C |
| ATOM | 2780 | CG2 | ILE | S | 806 | 32.267 | 21.765 | 38.255 | 1.00 | 66.46 | C |
| ATOM | 2781 | CD1 | ILE | S | 806 | 33.719 | 20.639 | 40.611 | 1.00 | 65.48 | C |
| ATOM | 2782 | N   | LEU | S | 813 | 29.912 | 8.313  | 36.265 | 1.00 | 60.30 | N |
| ATOM | 2783 | CA  | LEU | S | 813 | 30.605 | 8.781  | 35.059 | 1.00 | 60.57 | C |
| ATOM | 2784 | C   | LEU | S | 813 | 29.707 | 9.617  | 34.157 | 1.00 | 60.31 | C |
| ATOM | 2785 | O   | LEU | S | 813 | 28.484 | 9.496  | 34.194 | 1.00 | 60.27 | O |
| ATOM | 2786 | CB  | LEU | S | 813 | 31.167 | 7.599  | 34.266 | 1.00 | 60.46 | C |
| ATOM | 2787 | CG  | LEU | S | 813 | 32.067 | 6.674  | 35.092 | 1.00 | 60.30 | C |
| ATOM | 2788 | CD1 | LEU | S | 813 | 32.450 | 5.418  | 34.281 | 1.00 | 61.04 | C |
| ATOM | 2789 | CD2 | LEU | S | 813 | 33.301 | 7.421  | 35.602 | 1.00 | 59.11 | C |
| ATOM | 2790 | N   | GLN | S | 814 | 30.344 | 10.465 | 33.355 | 1.00 | 60.31 | N |
| ATOM | 2791 | CA  | GLN | S | 814 | 29.648 | 11.353 | 32.440 | 1.00 | 60.05 | C |
| ATOM | 2792 | C   | GLN | S | 814 | 30.557 | 11.803 | 31.295 | 1.00 | 59.62 | C |
| ATOM | 2793 | O   | GLN | S | 814 | 31.765 | 11.584 | 31.322 | 1.00 | 58.97 | O |
| ATOM | 2794 | CB  | GLN | S | 814 | 29.176 | 12.583 | 33.194 | 1.00 | 60.41 | C |
| ATOM | 2795 | CG  | GLN | S | 814 | 30.302 | 13.488 | 33.634 | 1.00 | 62.13 | C |
| ATOM | 2796 | CD  | GLN | S | 814 | 29.826 | 14.603 | 34.559 | 1.00 | 64.43 | C |
| ATOM | 2797 | OE1 | GLN | S | 814 | 29.260 | 14.327 | 35.616 | 1.00 | 65.48 | O |
| ATOM | 2798 | NE2 | GLN | S | 814 | 30.058 | 15.859 | 34.167 | 1.00 | 65.06 | N |
| ATOM | 2799 | N   | GLY | S | 815 | 29.960 | 12.456 | 30.302 | 1.00 | 59.55 | N |
| ATOM | 2800 | CA  | GLY | S | 815 | 30.675 | 12.927 | 29.136 | 1.00 | 59.21 | C |
| ATOM | 2801 | C   | GLY | S | 815 | 31.493 | 11.823 | 28.493 | 1.00 | 59.26 | C |
| ATOM | 2802 | O   | GLY | S | 815 | 31.049 | 10.678 | 28.399 | 1.00 | 58.48 | O |
| ATOM | 2803 | N   | GLU | S | 816 | 32.693 | 12.183 | 28.049 | 1.00 | 59.73 | N |
| ATOM | 2804 | CA  | GLU | S | 816 | 33.604 | 11.254 | 27.392 | 1.00 | 60.76 | C |
| ATOM | 2805 | C   | GLU | S | 816 | 33.768 | 9.941  | 28.168 | 1.00 | 61.61 | C |
| ATOM | 2806 | O   | GLU | S | 816 | 33.861 | 8.866  | 27.567 | 1.00 | 61.64 | O |
| ATOM | 2807 | CB  | GLU | S | 816 | 34.978 | 11.913 | 27.190 | 1.00 | 60.71 | C |
| ATOM | 2808 | CG  | GLU | S | 816 | 35.802 | 11.304 | 26.064 | 1.00 | 61.12 | C |
| ATOM | 2809 | CD  | GLU | S | 816 | 37.208 | 11.872 | 25.979 | 1.00 | 61.35 | C |
| ATOM | 2810 | OE1 | GLU | S | 816 | 38.066 | 11.370 | 26.730 | 1.00 | 61.67 | O |
| ATOM | 2811 | OE2 | GLU | S | 816 | 37.467 | 12.801 | 25.168 | 1.00 | 60.68 | O |
| ATOM | 2812 | N   | GLU | S | 817 | 33.791 | 10.030 | 29.495 | 1.00 | 62.56 | N |
| ATOM | 2813 | CA  | GLU | S | 817 | 33.962 | 8.851  | 30.332 | 1.00 | 63.66 | C |
| ATOM | 2814 | C   | GLU | S | 817 | 32.748 | 7.929  | 30.260 | 1.00 | 63.92 | C |
| ATOM | 2815 | O   | GLU | S | 817 | 32.887 | 6.709  | 30.187 | 1.00 | 63.68 | O |
| ATOM | 2816 | CB  | GLU | S | 817 | 34.217 | 9.257  | 31.777 | 1.00 | 63.99 | C |
| ATOM | 2817 | CG  | GLU | S | 817 | 35.518 | 10.012 | 31.974 | 1.00 | 65.72 | C |
| ATOM | 2818 | CD  | GLU | S | 817 | 35.371 | 11.514 | 31.786 | 1.00 | 69.17 | C |
| ATOM | 2819 | OE1 | GLU | S | 817 | 34.253 | 11.990 | 31.452 | 1.00 | 70.86 | O |
| ATOM | 2820 | OE2 | GLU | S | 817 | 36.384 | 12.228 | 31.984 | 1.00 | 71.76 | O |
| ATOM | 2821 | N   | LEU | S | 818 | 31.558 | 8.517  | 30.296 | 1.00 | 64.38 | N |
| ATOM | 2822 | CA  | LEU | S | 818 | 30.344 | 7.733  | 30.191 | 1.00 | 65.00 | C |
| ATOM | 2823 | C   | LEU | S | 818 | 30.367 | 6.935  | 28.890 | 1.00 | 65.31 | C |
| ATOM | 2824 | O   | LEU | S | 818 | 30.166 | 5.723  | 28.901 | 1.00 | 65.41 | O |
| ATOM | 2825 | CB  | LEU | S | 818 | 29.092 | 8.624  | 30.232 | 1.00 | 64.90 | C |
| ATOM | 2826 | CG  | LEU | S | 818 | 27.770 | 7.844  | 30.163 | 1.00 | 64.94 | C |

|        |      |     |     |       |     |        |        |        |      |       |    |
|--------|------|-----|-----|-------|-----|--------|--------|--------|------|-------|----|
| ATOM   | 2827 | CD1 | LEU | S     | 818 | 27.702 | 6.871  | 31.316 | 1.00 | 66.53 | C  |
| ATOM   | 2828 | CD2 | LEU | S     | 818 | 26.551 | 8.718  | 30.205 | 1.00 | 63.99 | C  |
| ATOM   | 2829 | N   | LEU | S     | 819 | 30.647 | 7.627  | 27.787 | 1.00 | 65.71 | N  |
| ATOM   | 2830 | CA  | LEU | S     | 819 | 30.608 | 7.037  | 26.445 | 1.00 | 66.10 | C  |
| ATOM   | 2831 | C   | LEU | S     | 819 | 31.569 | 5.851  | 26.294 | 1.00 | 66.37 | C  |
| ATOM   | 2832 | O   | LEU | S     | 819 | 31.174 | 4.773  | 25.852 | 1.00 | 65.86 | O  |
| ATOM   | 2833 | CB  | LEU | S     | 819 | 30.901 | 8.122  | 25.392 | 1.00 | 66.04 | C  |
| ATOM   | 2834 | CG  | LEU | S     | 819 | 30.860 | 7.737  | 23.916 | 1.00 | 66.00 | C  |
| ATOM   | 2835 | CD1 | LEU | S     | 819 | 29.537 | 7.149  | 23.501 | 1.00 | 66.14 | C  |
| ATOM   | 2836 | CD2 | LEU | S     | 819 | 31.162 | 8.967  | 23.083 | 1.00 | 67.31 | C  |
| ATOM   | 2837 | N   | ARG | S     | 820 | 32.820 | 6.053  | 26.684 | 1.00 | 66.68 | N  |
| ATOM   | 2838 | CA  | ARG | S     | 820 | 33.824 | 5.013  | 26.561 | 1.00 | 67.34 | C  |
| ATOM   | 2839 | C   | ARG | S     | 820 | 33.492 | 3.801  | 27.432 | 1.00 | 67.41 | C  |
| ATOM   | 2840 | O   | ARG | S     | 820 | 33.573 | 2.643  | 26.969 | 1.00 | 67.19 | O  |
| ATOM   | 2841 | CB  | ARG | S     | 820 | 35.196 | 5.574  | 26.917 | 1.00 | 67.66 | C  |
| ATOM   | 2842 | CG  | ARG | S     | 820 | 35.628 | 6.605  | 25.907 | 1.00 | 69.12 | C  |
| ATOM   | 2843 | CD  | ARG | S     | 820 | 37.048 | 7.061  | 26.030 | 1.00 | 71.00 | C  |
| ATOM   | 2844 | NE  | ARG | S     | 820 | 37.309 | 8.138  | 25.079 | 1.00 | 73.46 | N  |
| ATOM   | 2845 | CZ  | ARG | S     | 820 | 38.442 | 8.839  | 25.014 | 1.00 | 75.31 | C  |
| ATOM   | 2846 | NH1 | ARG | S     | 820 | 39.451 | 8.581  | 25.851 | 1.00 | 75.90 | N  |
| ATOM   | 2847 | NH2 | ARG | S     | 820 | 38.566 | 9.806  | 24.104 | 1.00 | 75.55 | N  |
| ATOM   | 2848 | N   | ALA | S     | 821 | 33.118 | 4.067  | 28.684 | 1.00 | 67.11 | N  |
| ATOM   | 2849 | CA  | ALA | S     | 821 | 32.712 | 2.999  | 29.580 | 1.00 | 66.99 | C  |
| ATOM   | 2850 | C   | ALA | S     | 821 | 31.609 | 2.171  | 28.898 | 1.00 | 66.76 | C  |
| ATOM   | 2851 | O   | ALA | S     | 821 | 31.660 | 0.945  | 28.889 | 1.00 | 66.63 | O  |
| ATOM   | 2852 | CB  | ALA | S     | 821 | 32.234 | 3.562  | 30.901 | 1.00 | 66.88 | C  |
| ATOM   | 2853 | N   | LEU | S     | 822 | 30.625 | 2.851  | 28.313 | 1.00 | 66.58 | N  |
| ATOM   | 2854 | CA  | LEU | S     | 822 | 29.538 | 2.173  | 27.607 | 1.00 | 66.36 | C  |
| ATOM   | 2855 | C   | LEU | S     | 822 | 30.027 | 1.439  | 26.359 | 1.00 | 66.21 | C  |
| ATOM   | 2856 | O   | LEU | S     | 822 | 29.429 | 0.444  | 25.956 | 1.00 | 66.11 | O  |
| ATOM   | 2857 | CB  | LEU | S     | 822 | 28.451 | 3.172  | 27.223 | 1.00 | 66.06 | C  |
| ATOM   | 2858 | CG  | LEU | S     | 822 | 27.710 | 3.789  | 28.406 | 1.00 | 65.45 | C  |
| ATOM   | 2859 | CD1 | LEU | S     | 822 | 26.559 | 4.613  | 27.885 | 1.00 | 65.37 | C  |
| ATOM   | 2860 | CD2 | LEU | S     | 822 | 27.213 | 2.732  | 29.396 | 1.00 | 65.08 | C  |
| TER    | 2861 |     | LEU | S     | 822 |        |        |        |      |       |    |
| HETATM | 2862 | ZN  | ZN  | A1350 |     | 23.324 | 27.578 | 28.817 | 1.00 | 32.29 | ZN |
| HETATM | 2863 | C1  | OGA | A1351 |     | 22.262 | 25.308 | 27.891 | 1.00 | 34.79 | C  |
| HETATM | 2864 | C2  | OGA | A1351 |     | 21.209 | 25.940 | 28.487 | 1.00 | 32.90 | C  |
| HETATM | 2865 | C4  | OGA | A1351 |     | 18.882 | 25.730 | 29.253 | 1.00 | 32.24 | C  |
| HETATM | 2866 | C5  | OGA | A1351 |     | 17.543 | 25.251 | 28.735 | 1.00 | 32.20 | C  |
| HETATM | 2867 | O1  | OGA | A1351 |     | 22.091 | 24.207 | 27.399 | 1.00 | 33.47 | O  |
| HETATM | 2868 | O2  | OGA | A1351 |     | 23.404 | 25.817 | 27.813 | 1.00 | 33.83 | O  |
| HETATM | 2869 | O2' | OGA | A1351 |     | 21.299 | 27.077 | 29.004 | 1.00 | 31.02 | O  |
| HETATM | 2870 | O3  | OGA | A1351 |     | 17.430 | 24.476 | 27.795 | 1.00 | 33.67 | O  |
| HETATM | 2871 | N1  | OGA | A1351 |     | 20.067 | 25.271 | 28.520 | 1.00 | 29.83 | N  |
| HETATM | 2872 | O4  | OGA | A1351 |     | 16.551 | 25.641 | 29.307 | 1.00 | 32.21 | O  |
| HETATM | 2873 | S   | SO4 | A1352 |     | 0.290  | 25.194 | 43.827 | 1.00 | 90.02 | S  |
| HETATM | 2874 | O1  | SO4 | A1352 |     | 1.120  | 26.025 | 44.689 | 1.00 | 89.95 | O  |
| HETATM | 2875 | O2  | SO4 | A1352 |     | 1.151  | 24.261 | 43.106 | 1.00 | 88.91 | O  |
| HETATM | 2876 | O3  | SO4 | A1352 |     | -0.627 | 24.447 | 44.672 | 1.00 | 90.38 | O  |
| HETATM | 2877 | O4  | SO4 | A1352 |     | -0.468 | 26.028 | 42.891 | 1.00 | 89.30 | O  |
| HETATM | 2878 | S   | SO4 | A1353 |     | 1.893  | 28.515 | 29.870 | 1.00 | 98.62 | S  |
| HETATM | 2879 | O1  | SO4 | A1353 |     | 3.138  | 29.102 | 30.350 | 1.00 | 97.69 | O  |
| HETATM | 2880 | O2  | SO4 | A1353 |     | 2.145  | 27.399 | 28.947 | 1.00 | 97.91 | O  |
| HETATM | 2881 | O3  | SO4 | A1353 |     | 1.205  | 28.059 | 31.078 | 1.00 | 99.26 | O  |
| HETATM | 2882 | O4  | SO4 | A1353 |     | 1.078  | 29.515 | 29.171 | 1.00 | 98.46 | O  |
| HETATM | 2883 | O   | HOH | H     | 1   | 38.820 | 33.858 | 31.965 | 1.00 | 46.43 | O  |
| HETATM | 2884 | O   | HOH | H     | 2   | 33.795 | 30.509 | 39.255 | 1.00 | 71.93 | O  |
| HETATM | 2885 | O   | HOH | H     | 3   | 34.891 | 30.536 | 35.372 | 1.00 | 48.26 | O  |
| HETATM | 2886 | O   | HOH | H     | 4   | 35.615 | 13.844 | 24.220 | 1.00 | 48.67 | O  |
| HETATM | 2887 | O   | HOH | Z     | 1   | 11.592 | 21.463 | 13.878 | 1.00 | 49.06 | O  |



|        |      |   |     |   |    |        |        |        |      |       |   |
|--------|------|---|-----|---|----|--------|--------|--------|------|-------|---|
| HETATM | 2888 | O | HOH | Z | 2  | 9.700  | 21.662 | 12.247 | 1.00 | 70.56 | O |
| HETATM | 2889 | O | HOH | Z | 3  | 1.136  | 21.407 | 7.962  | 1.00 | 66.59 | O |
| HETATM | 2890 | O | HOH | Z | 4  | 2.407  | 19.370 | 5.351  | 1.00 | 60.28 | O |
| HETATM | 2891 | O | HOH | Z | 5  | 1.014  | 29.292 | 13.196 | 1.00 | 61.25 | O |
| HETATM | 2892 | O | HOH | Z | 6  | 2.256  | 32.365 | 14.166 | 1.00 | 73.91 | O |
| HETATM | 2893 | O | HOH | Z | 7  | 11.526 | 44.954 | 15.330 | 1.00 | 68.94 | O |
| HETATM | 2894 | O | HOH | Z | 8  | -1.438 | 30.257 | 22.663 | 1.00 | 85.46 | O |
| HETATM | 2895 | O | HOH | Z | 9  | 7.738  | 30.579 | 27.736 | 1.00 | 46.83 | O |
| HETATM | 2896 | O | HOH | Z | 10 | 3.543  | 32.597 | 32.323 | 1.00 | 73.21 | O |
| HETATM | 2897 | O | HOH | Z | 11 | 6.618  | 43.722 | 26.114 | 1.00 | 79.20 | O |
| HETATM | 2898 | O | HOH | Z | 12 | 4.723  | 37.184 | 27.600 | 1.00 | 69.48 | O |
| HETATM | 2899 | O | HOH | Z | 13 | 10.942 | 35.610 | 30.382 | 1.00 | 48.93 | O |
| HETATM | 2900 | O | HOH | Z | 14 | 13.888 | 48.615 | 19.570 | 1.00 | 55.60 | O |
| HETATM | 2901 | O | HOH | Z | 15 | 12.153 | 41.664 | 15.818 | 1.00 | 61.09 | O |
| HETATM | 2902 | O | HOH | Z | 16 | 15.898 | 30.602 | 12.921 | 1.00 | 48.84 | O |
| HETATM | 2903 | O | HOH | Z | 17 | 13.629 | 22.042 | 7.314  | 1.00 | 56.45 | O |
| HETATM | 2904 | O | HOH | Z | 18 | 14.608 | 26.242 | 13.702 | 1.00 | 55.84 | O |
| HETATM | 2905 | O | HOH | Z | 19 | 21.110 | 23.978 | 3.732  | 1.00 | 49.91 | O |
| HETATM | 2906 | O | HOH | Z | 20 | 22.517 | 24.246 | 0.061  | 1.00 | 58.70 | O |
| HETATM | 2907 | O | HOH | Z | 21 | 27.322 | 30.745 | 5.813  | 1.00 | 71.25 | O |
| HETATM | 2908 | O | HOH | Z | 22 | 26.669 | 21.831 | 43.291 | 1.00 | 84.79 | O |
| HETATM | 2909 | O | HOH | Z | 23 | 36.928 | 29.423 | 21.116 | 1.00 | 60.53 | O |
| HETATM | 2910 | O | HOH | Z | 24 | 28.560 | 37.933 | 15.396 | 1.00 | 65.84 | O |
| HETATM | 2911 | O | HOH | Z | 25 | 29.717 | 37.018 | 10.091 | 1.00 | 70.57 | O |
| HETATM | 2912 | O | HOH | Z | 26 | 19.889 | 17.921 | 13.411 | 1.00 | 40.68 | O |
| HETATM | 2913 | O | HOH | Z | 27 | 18.190 | 15.068 | 13.047 | 1.00 | 45.64 | O |
| HETATM | 2914 | O | HOH | Z | 28 | 19.229 | 14.479 | 16.581 | 1.00 | 44.23 | O |
| HETATM | 2915 | O | HOH | Z | 29 | 5.509  | 12.781 | 28.209 | 1.00 | 48.58 | O |
| HETATM | 2916 | O | HOH | Z | 30 | 19.118 | 6.397  | 36.829 | 1.00 | 62.79 | O |
| HETATM | 2917 | O | HOH | Z | 31 | 33.446 | 44.026 | 25.377 | 1.00 | 68.72 | O |
| HETATM | 2918 | O | HOH | Z | 32 | 8.427  | 26.875 | 44.426 | 1.00 | 65.85 | O |
| HETATM | 2919 | O | HOH | Z | 33 | 9.122  | 31.413 | 42.815 | 1.00 | 79.14 | O |
| HETATM | 2920 | O | HOH | Z | 34 | 15.645 | 37.855 | 35.686 | 1.00 | 55.81 | O |
| HETATM | 2921 | O | HOH | Z | 35 | 16.264 | 30.912 | 40.283 | 1.00 | 52.67 | O |
| HETATM | 2922 | O | HOH | Z | 36 | 28.580 | 24.804 | 42.231 | 1.00 | 71.47 | O |
| HETATM | 2923 | O | HOH | Z | 37 | 25.125 | 24.702 | 42.513 | 1.00 | 61.76 | O |
| HETATM | 2924 | O | HOH | Z | 38 | 31.710 | 33.903 | 46.336 | 1.00 | 58.86 | O |
| HETATM | 2925 | O | HOH | Z | 39 | 24.430 | 38.695 | 49.842 | 1.00 | 64.87 | O |
| HETATM | 2926 | O | HOH | Z | 40 | 21.999 | 17.349 | 48.274 | 1.00 | 78.90 | O |
| HETATM | 2927 | O | HOH | Z | 41 | 22.174 | 10.277 | 34.700 | 1.00 | 61.90 | O |
| HETATM | 2928 | O | HOH | Z | 42 | 17.917 | -1.798 | 33.038 | 1.00 | 69.51 | O |
| HETATM | 2929 | O | HOH | Z | 43 | 36.654 | 10.887 | 7.525  | 1.00 | 72.57 | O |
| HETATM | 2930 | O | HOH | Z | 44 | 13.628 | 20.833 | 28.536 | 1.00 | 46.20 | O |
| HETATM | 2931 | O | HOH | Z | 45 | 3.910  | 21.434 | 31.018 | 1.00 | 60.17 | O |
| HETATM | 2932 | O | HOH | Z | 46 | 30.778 | 38.131 | 33.414 | 1.00 | 33.59 | O |
| HETATM | 2933 | O | HOH | Z | 47 | 25.976 | 26.458 | 26.213 | 1.00 | 38.20 | O |
| HETATM | 2934 | O | HOH | Z | 48 | 35.876 | 25.491 | 27.760 | 1.00 | 47.36 | O |
| HETATM | 2935 | O | HOH | Z | 49 | 36.704 | 26.679 | 21.111 | 1.00 | 49.53 | O |
| HETATM | 2936 | O | HOH | Z | 50 | 17.375 | 16.970 | 18.001 | 1.00 | 37.06 | O |
| HETATM | 2937 | O | HOH | Z | 51 | 5.442  | 16.762 | 21.954 | 1.00 | 48.45 | O |
| HETATM | 2938 | O | HOH | Z | 52 | 6.786  | 12.615 | 22.641 | 1.00 | 71.97 | O |
| HETATM | 2939 | O | HOH | Z | 53 | 7.201  | 17.017 | 20.359 | 1.00 | 48.19 | O |
| HETATM | 2940 | O | HOH | Z | 54 | 6.512  | 22.748 | 23.330 | 1.00 | 52.43 | O |
| HETATM | 2941 | O | HOH | Z | 55 | 29.528 | 38.794 | 26.547 | 1.00 | 33.74 | O |
| HETATM | 2942 | O | HOH | Z | 56 | 30.683 | 39.271 | 19.412 | 1.00 | 42.04 | O |
| HETATM | 2943 | O | HOH | Z | 57 | 26.571 | 42.213 | 18.009 | 1.00 | 59.45 | O |
| HETATM | 2944 | O | HOH | Z | 58 | 29.038 | 40.259 | 16.007 | 1.00 | 65.33 | O |
| HETATM | 2945 | O | HOH | Z | 59 | 27.631 | 44.557 | 31.407 | 1.00 | 36.71 | O |
| HETATM | 2946 | O | HOH | Z | 60 | 27.654 | 48.738 | 30.067 | 1.00 | 46.82 | O |
| HETATM | 2947 | O | HOH | Z | 61 | 30.426 | 45.052 | 25.424 | 1.00 | 49.55 | O |
| HETATM | 2948 | O | HOH | Z | 62 | 25.946 | 50.745 | 30.903 | 1.00 | 51.76 | O |



[illegible]

Structure 4

Below are the coordinates for structure 4 (the 2.85 Å structure of FIH:Fe(II):2OG):

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HEADER      TRANSCRIPTION ACTIVATOR/INHIBITOR          12-AUG-02   1H2N
TITLE       FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE       2 FRAGMENT PEPTIDE
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND      3 SYNONYM: FIH1;
COMPND      4 CHAIN: A;
COMPND      5 ENGINEERED: YES
SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE      3 ORGANISM_COMMON: HUMAN;
SOURCE      4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE      5 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE      6 EXPRESSION_SYSTEM_PLASMID: PET28A(+)
KEYWDS      FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
KEYWDS      2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE
EXPDTA      X-RAY DIFFRACTION
AUTHOR      J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,I.SCHLEMMINGER,
AUTHOR      2 J.F.SEIBEL,C.J.SCHOFIELD
REVDAT      1   04-SEP-02 1H2N   0
JRNL        AUTH   J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,
JRNL        AUTH 2 I.SCHLEMMINGER,J.F.SEIBEL,C.J.SCHOFIELD
JRNL        TITL   FIH:HIF-FRAGMENT COMPLEXES
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK      2
REMARK      2 RESOLUTION. 2.84 ANGSTROMS.
REMARK      3
REMARK      3 REFINEMENT.
REMARK      3   PROGRAM       : REFMAC 5.0
REMARK      3   AUTHORS        : MURSHUDOV,VAGIN,DODSON
REMARK      3
REMARK      3   REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK      3
REMARK      3 DATA USED IN REFINEMENT.
REMARK      3   RESOLUTION RANGE HIGH (ANGSTROMS) :   2.84
REMARK      3   RESOLUTION RANGE LOW  (ANGSTROMS) :  30.00
REMARK      3   DATA CUTOFF          (SIGMA(F)) :  NONE
REMARK      3   COMPLETENESS FOR RANGE       (%) :  99.51
REMARK      3   NUMBER OF REFLECTIONS           :  12577
REMARK      3
REMARK      3 FIT TO DATA USED IN REFINEMENT.
REMARK      3   CROSS-VALIDATION METHOD               : THROUGHOUT
REMARK      3   FREE R VALUE TEST SET SELECTION          : RANDOM
REMARK      3   R VALUE             (WORKING + TEST SET) : 0.23287
REMARK      3   R VALUE             (WORKING SET)           : 0.23094
REMARK      3   FREE R VALUE                               : 0.25695
REMARK      3   FREE R VALUE TEST SET SIZE      (%) :   7.7
REMARK      3   FREE R VALUE TEST SET COUNT        :  1046
REMARK      3
REMARK      3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK      3   TOTAL NUMBER OF BINS USED                   :    20
REMARK      3   BIN RESOLUTION RANGE HIGH                   :   2.840
REMARK      3   BIN RESOLUTION RANGE LOW                    :   2.913
REMARK      3   REFLECTION IN BIN      (WORKING SET)         :    828

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REMARK 3   BIN R VALUE (WORKING SET) : 0.286
REMARK 3   BIN FREE R VALUE SET COUNT : 81
REMARK 3   BIN FREE R VALUE : 0.315
REMARK 3
REMARK 3   NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3   PROTEIN ATOMS : 2689
REMARK 3   NUCLEIC ACID ATOMS : 0
REMARK 3   HETEROGEN ATOMS : 26
REMARK 3   SOLVENT ATOMS : 3
REMARK 3
REMARK 3   B VALUES.
REMARK 3   FROM WILSON PLOT (A**2) : NULL
REMARK 3   MEAN B VALUE (OVERALL, A**2) : 35.345
REMARK 3   OVERALL ANISOTROPIC B VALUE.
REMARK 3   B11 (A**2) : -1.02
REMARK 3   B22 (A**2) : -1.02
REMARK 3   B33 (A**2) : 2.03
REMARK 3   B12 (A**2) : 0.00
REMARK 3   B13 (A**2) : 0.00
REMARK 3   B23 (A**2) : 0.00
REMARK 3
REMARK 3   ESTIMATED OVERALL COORDINATE ERROR.
REMARK 3   ESU BASED ON R VALUE (A): 0.852
REMARK 3   ESU BASED ON FREE R VALUE (A): 0.349
REMARK 3   ESU BASED ON MAXIMUM LIKELIHOOD (A): 0.398
REMARK 3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 19.679
REMARK 3
REMARK 3   CORRELATION COEFFICIENTS.
REMARK 3   CORRELATION COEFFICIENT FO-FC : 0.913
REMARK 3   CORRELATION COEFFICIENT FO-FC FREE : 0.901
REMARK 3
REMARK 3   RMS DEVIATIONS FROM IDEAL VALUES COUNT RMS WEIGHT
REMARK 3   BOND LENGTHS REFINED ATOMS (A): 2791 ; 0.015 ; 0.021
REMARK 3   BOND LENGTHS OTHERS (A): 2388 ; 0.001 ; 0.020
REMARK 3   BOND ANGLES REFINED ATOMS (DEGREES): 3799 ; 1.628 ; 1.945
REMARK 3   BOND ANGLES OTHERS (DEGREES): 5576 ; 0.823 ; 3.000
REMARK 3   TORSION ANGLES, PERIOD 1 (DEGREES): 330 ; 4.268 ; 3.000
REMARK 3   TORSION ANGLES, PERIOD 3 (DEGREES): 479 ; 18.082 ; 15.000
REMARK 3   CHIRAL-CENTER RESTRAINTS (A**3): 384 ; 0.095 ; 0.200
REMARK 3   GENERAL PLANES REFINED ATOMS (A): 3137 ; 0.005 ; 0.020
REMARK 3   GENERAL PLANES OTHERS (A): 575 ; 0.002 ; 0.020
REMARK 3   NON-BONDED CONTACTS REFINED ATOMS (A): 717 ; 0.255 ; 0.300
REMARK 3   NON-BONDED CONTACTS OTHERS (A): 2425 ; 0.224 ; 0.300
REMARK 3   H-BOND (X...Y) REFINED ATOMS (A): 165 ; 0.139 ; 0.500
REMARK 3   H-BOND (X...Y) OTHERS (A): 1 ; 0.102 ; 0.500
REMARK 3   POTENTIAL METAL-ION REFINED ATOMS (A): 3 ; 0.112 ; 0.500
REMARK 3   SYMMETRY VDW REFINED ATOMS (A): 14 ; 0.256 ; 0.300
REMARK 3   SYMMETRY VDW OTHERS (A): 62 ; 0.273 ; 0.300
REMARK 3   SYMMETRY H-BOND REFINED ATOMS (A): 4 ; 0.214 ; 0.500
REMARK 3   SYMMETRY H-BOND OTHERS (A): 1 ; 0.061 ; 0.500
REMARK 3
REMARK 3   ISOTROPIC THERMAL FACTOR RESTRAINTS. COUNT RMS WEIGHT
REMARK 3   MAIN-CHAIN BOND REFINED ATOMS (A**2): 1659 ; 0.312 ; 1.500
REMARK 3   MAIN-CHAIN ANGLE REFINED ATOMS (A**2): 2675 ; 0.598 ; 2.000
REMARK 3   SIDE-CHAIN BOND REFINED ATOMS (A**2): 1132 ; 1.058 ; 3.000
REMARK 3   SIDE-CHAIN ANGLE REFINED ATOMS (A**2): 1124 ; 1.795 ; 4.500
REMARK 3
REMARK 3   NCS RESTRAINTS STATISTICS
REMARK 3   NUMBER OF NCS GROUPS : NULL
REMARK 3
REMARK 3   TLS DETAILS

```

REMARK 3 NUMBER OF TLS GROUPS : 1  
REMARK 3  
REMARK 3 TLS GROUP : 1  
REMARK 3 NUMBER OF COMPONENTS GROUP : 1  
REMARK 3 COMPONENTS C SSSEQI TO C SSSEQI  
REMARK 3 RESIDUE RANGE : A 15 A 452  
REMARK 3 ORIGIN FOR THE GROUP (A): 21.4490 27.4200 27.7870  
REMARK 3 T TENSOR  
REMARK 3 T11: 0.2230 T22: 0.0562  
REMARK 3 T33: 0.0967 T12: 0.0111  
REMARK 3 T13: -0.0923 T23: 0.0525  
REMARK 3 L TENSOR  
REMARK 3 L11: 1.6842 L22: 4.4489  
REMARK 3 L33: 2.0658 L12: 1.5597  
REMARK 3 L13: 1.1572 L23: 2.3523  
REMARK 3 S TENSOR  
REMARK 3 S11: 0.1098 S12: -0.2106 S13: -0.0766  
REMARK 3 S21: 0.3449 S22: -0.0455 S23: 0.2455  
REMARK 3 S31: 0.3515 S32: -0.1199 S33: -0.0643  
REMARK 3  
REMARK 3 BULK SOLVENT MODELLING.  
REMARK 3 METHOD USED : BABINET MODEL WITH MASK  
REMARK 3 PARAMETERS FOR MASK CALCULATION  
REMARK 3 VDW PROBE RADIUS : 1.40  
REMARK 3 ION PROBE RADIUS : 0.80  
REMARK 3 SHRINKAGE RADIUS : 0.80  
REMARK 3  
REMARK 3 OTHER REFINEMENT REMARKS: SEE REMARK 400  
REMARK 4  
REMARK 4 1H2N COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998  
REMARK 100  
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.  
REMARK 100 THE EBI ID CODE IS EBI-11174.  
REMARK 200  
REMARK 200 EXPERIMENTAL DETAILS  
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION  
REMARK 200 DATE OF DATA COLLECTION : 15-MAY-2002  
REMARK 200 TEMPERATURE (KELVIN) : 100  
REMARK 200 PH : 7.5  
REMARK 200 NUMBER OF CRYSTALS USED : 1  
REMARK 200  
REMARK 200 SYNCHROTRON (Y/N) : Y  
REMARK 200 RADIATION SOURCE : SRS BEAMLINE PX9.5  
REMARK 200 BEAMLINE : PX9.5  
REMARK 200 X-RAY GENERATOR MODEL : NULL  
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M  
REMARK 200 WAVELENGTH OR RANGE (A) : 0.92  
REMARK 200 MONOCHROMATOR : NULL  
REMARK 200 OPTICS : NULL  
REMARK 200  
REMARK 200 DETECTOR TYPE : MARCCD  
REMARK 200 DETECTOR MANUFACTURER : MARRESEARCH  
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : MOSFLM  
REMARK 200 DATA SCALING SOFTWARE : SCALA  
REMARK 200  
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 13703  
REMARK 200 RESOLUTION RANGE HIGH (A) : 2.84  
REMARK 200 RESOLUTION RANGE LOW (A) : 34.1  
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NONE  
REMARK 200  
REMARK 200 OVERALL.



REMARK 200 COMPLETENESS FOR RANGE (%) : 99.2  
 REMARK 200 DATA REDUNDANCY : 6.7  
 REMARK 200 R MERGE (I) : 0.067  
 REMARK 200 R SYM (I) : NULL  
 REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 9.4  
 REMARK 200  
 REMARK 200 IN THE HIGHEST RESOLUTION SHELL.  
 REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.84  
 REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A) : 2.99  
 REMARK 200 COMPLETENESS FOR SHELL (%) : 94.9  
 REMARK 200 DATA REDUNDANCY IN SHELL : 5.2  
 REMARK 200 R MERGE FOR SHELL (I) : 0.309  
 REMARK 200 R SYM FOR SHELL (I) : NULL  
 REMARK 200 <I/SIGMA(I)> FOR SHELL : 2.4  
 REMARK 200  
 REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH  
 REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT  
 REMARK 200 SOFTWARE USED: NULL  
 REMARK 200 STARTING MODEL: NULL  
 REMARK 200  
 REMARK 200 REMARK: SEE REMARK 400  
 REMARK 280  
 REMARK 280 CRYSTAL  
 REMARK 280 SOLVENT CONTENT, VS (%): 63  
 REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS\*\*3/DA): 3.4  
 REMARK 280  
 REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE,  
 REMARK 280 4% PEG400, 0.1M HEPES PH7.5 ARGON ATMOSPHERE,  
 REMARK 280 11MG/ML PROTEIN WITH 1MM FE(II), 2.5MM AKG AND 2.5MM  
 REMARK 280 PEPTIDE (SEE REMARK 400)  
 REMARK 290  
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY  
 REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2  
 REMARK 290  

| SYNOP  | SYMMETRY            |
|--------|---------------------|
| NNNMMM | OPERATOR            |
| 1555   | X, Y, Z             |
| 2555   | -X, -Y, 1/2+Z       |
| 3555   | 1/2-Y, 1/2+X, 1/4+Z |
| 4555   | 1/2+Y, 1/2-X, 3/4+Z |
| 5555   | 1/2-X, 1/2+Y, 1/4-Z |
| 6555   | 1/2+X, 1/2-Y, 3/4-Z |
| 7555   | Y, X, -Z            |
| 8555   | -Y, -X, 1/2-Z       |

 REMARK 290  
 REMARK 290 WHERE NNN -> OPERATOR NUMBER  
 REMARK 290 MMM -> TRANSLATION VECTOR  
 REMARK 290  
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS  
 REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM  
 REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY  
 REMARK 290 RELATED MOLECULES.  

| SMTRY1 | 1 | 1.000000  | 0.000000  | 0.000000 | 0.000000 |
|--------|---|-----------|-----------|----------|----------|
| SMTRY2 | 1 | 0.000000  | 1.000000  | 0.000000 | 0.000000 |
| SMTRY3 | 1 | 0.000000  | 0.000000  | 1.000000 | 0.000000 |
| SMTRY1 | 2 | -1.000000 | 0.000000  | 0.000000 | 0.000000 |
| SMTRY2 | 2 | 0.000000  | -1.000000 | 0.000000 | 0.000000 |
| SMTRY3 | 2 | 0.000000  | 0.000000  | 1.000000 | 73.36600 |
| SMTRY1 | 3 | 0.000000  | -1.000000 | 0.000000 | 43.17100 |
| SMTRY2 | 3 | 1.000000  | 0.000000  | 0.000000 | 43.17100 |
| SMTRY3 | 3 | 0.000000  | 0.000000  | 1.000000 | 36.68300 |

|            |  |   |           |           |           |           |
|------------|--|---|-----------|-----------|-----------|-----------|
| REMARK 290 | SMTRY1   | 4 | 0.000000  | 1.000000  | 0.000000  | 43.17100  |
| REMARK 290 | SMTRY2   | 4 | -1.000000 | 0.000000  | 0.000000  | 43.17100  |
| REMARK 290 | SMTRY3   | 4 | 0.000000  | 0.000000  | 1.000000  | 110.04900 |
| REMARK 290 | SMTRY1   | 5 | -1.000000 | 0.000000  | 0.000000  | 43.17100  |
| REMARK 290 | SMTRY2   | 5 | 0.000000  | 1.000000  | 0.000000  | 43.17100  |
| REMARK 290 | SMTRY3   | 5 | 0.000000  | 0.000000  | -1.000000 | 36.68300  |
| REMARK 290 | SMTRY1   | 6 | 1.000000  | 0.000000  | 0.000000  | 43.17100  |
| REMARK 290 | SMTRY2   | 6 | 0.000000  | -1.000000 | 0.000000  | 43.17100  |
| REMARK 290 | SMTRY3   | 6 | 0.000000  | 0.000000  | -1.000000 | 110.04900 |
| REMARK 290 | SMTRY1   | 7 | 0.000000  | 1.000000  | 0.000000  | 0.00000   |
| REMARK 290 | SMTRY2   | 7 | 1.000000  | 0.000000  | 0.000000  | 0.00000   |
| REMARK 290 | SMTRY3   | 7 | 0.000000  | 0.000000  | -1.000000 | 0.00000   |
| REMARK 290 | SMTRY1   | 8 | 0.000000  | -1.000000 | 0.000000  | 0.00000   |
| REMARK 290 | SMTRY2   | 8 | -1.000000 | 0.000000  | 0.000000  | 0.00000   |
| REMARK 290 | SMTRY3   | 8 | 0.000000  | 0.000000  | -1.000000 | 73.36600  |
| REMARK 290 |  |   |           |           |           |           |
| REMARK 290 | REMARK: NULL   |   |           |           |           |           |
| REMARK 300 |  |   |           |           |           |           |
| REMARK 300 | BIOMOLECULE: 1   |   |           |           |           |           |
| REMARK 300 | THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT       |   |           |           |           |           |
| REMARK 300 | WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR               |   |           |           |           |           |
| REMARK 300 | INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).          |   |           |           |           |           |
| REMARK 300 |  |   |           |           |           |           |
| REMARK 300 | QUATERNARY STRUCTURE FOR THIS ENTRY: DIMERIC                   |   |           |           |           |           |
| REMARK 300 |  |   |           |           |           |           |
| REMARK 300 | THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.                  |   |           |           |           |           |
| REMARK 300 |  |   |           |           |           |           |
| REMARK 300 | FOR THE HOMO-ASSEMBLY DESCRIBED BY REMARK 350                  |   |           |           |           |           |
| REMARK 300 | THE DIFFERENCE IN ACCESSIBLE SURFACE AREA PER                  |   |           |           |           |           |
| REMARK 300 | CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR                  |   |           |           |           |           |
| REMARK 300 | THE CHAIN IN THE COMPLEX IS 1600.4 ANGSTROM**2                 |   |           |           |           |           |
| REMARK 350 |  |   |           |           |           |           |
| REMARK 350 | GENERATING THE BIOMOLECULE                                     |   |           |           |           |           |
| REMARK 350 | COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN     |   |           |           |           |           |
| REMARK 350 | BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE          |   |           |           |           |           |
| REMARK 350 | MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS    |   |           |           |           |           |
| REMARK 350 | GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND                     |   |           |           |           |           |
| REMARK 350 | CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.                         |   |           |           |           |           |
| REMARK 350 |  |   |           |           |           |           |
| REMARK 350 | BIOMOLECULE: 1   |   |           |           |           |           |
| REMARK 350 | APPLY THE FOLLOWING TO CHAINS: A                               |   |           |           |           |           |
| REMARK 350 | BIOMT1   | 1 | 1.000000  | 0.000000  | 0.000000  | 0.00000   |
| REMARK 350 | BIOMT2   | 1 | 0.000000  | 1.000000  | 0.000000  | 0.00000   |
| REMARK 350 | BIOMT3   | 1 | 0.000000  | 0.000000  | 1.000000  | 0.00000   |
| REMARK 350 | BIOMT1   | 2 | 0.000000  | -1.000000 | 0.000000  | 86.34200  |
| REMARK 350 | BIOMT2   | 2 | -1.000000 | 0.000000  | 0.000000  | 86.34200  |
| REMARK 350 | BIOMT3   | 2 | 0.000000  | 0.000000  | -1.000000 | 73.36600  |
| REMARK 400 |  |   |           |           |           |           |
| REMARK 400 | COMPOUND   |   |           |           |           |           |
| REMARK 400 |  |   |           |           |           |           |
| REMARK 400 | THE PROTEIN (CHAIN A) WAS CRYSTALLIZED IN THE PRESENCE         |   |           |           |           |           |
| REMARK 400 | OF A PEPTIDE FRAGMENT FROM ENDOTHELIAL PAS DOMAIN PROTEIN 1    |   |           |           |           |           |
| REMARK 400 | SWISS-PROT ID Q99814 (RESIDUES 846-858) BUT NONE OF THE        |   |           |           |           |           |
| REMARK 400 | RESIDUES CORRESPONDING TO THE PEPTIDE WERE VISIBLE IN THE      |   |           |           |           |           |
| REMARK 400 | ELECTRON DENSITY MAPS. IT IS POSSIBLE THAT THE PEPTIDE DID     |   |           |           |           |           |
| REMARK 400 | NOT BIND TO THE PROTEIN AND HENCE HAS NOT BEEN INCLUDED IN THE |   |           |           |           |           |
| REMARK 400 | COMPND, SOURCE AND SEQRES RECORDS.                             |   |           |           |           |           |
| REMARK 400 |  |   |           |           |           |           |
| REMARK 400 | THE SEQUENCE OF THE FRAGMENT IS GIVEN BELOW.                   |   |           |           |           |           |
| REMARK 400 |  |   |           |           |           |           |
| REMARK 400 | VAL ASN VAL PRO VAL LEU GLY SER SER THR LEU LEU GLN            |   |           |           |           |           |

REMARK 465  
REMARK 465 MISSING RESIDUES  
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE  
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN  
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)  
REMARK 465  
REMARK 465 M RES C SSSEQI  
REMARK 465 MET A 1  
REMARK 465 ALA A 2  
REMARK 465 ALA A 3  
REMARK 465 THR A 4  
REMARK 465 ALA A 5  
REMARK 465 ALA A 6  
REMARK 465 GLU A 7  
REMARK 465 ALA A 8  
REMARK 465 VAL A 9  
REMARK 465 ALA A 10  
REMARK 465 SER A 11  
REMARK 465 GLY A 12  
REMARK 465 SER A 13  
REMARK 465 GLY A 14  
REMARK 465 LYS A 304  
REMARK 465 ARG A 305  
REMARK 465 ILE A 306  
REMARK 470  
REMARK 470 MISSING ATOM  
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;  
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;  
REMARK 470 I=INSERTION CODE):  
REMARK 470 M RES CSSEQI ATOMS  
REMARK 470 GLU A 15 CG CD OE1 OE2  
REMARK 470 GLU A 29 CG CD OE1 OE2  
REMARK 470 ASN A 87 CG OD1 ND2  
REMARK 470 LYS A 106 CD CE NZ  
REMARK 470 LYS A 115 CG CD CE NZ  
REMARK 470 ARG A 117 CG CD NE CZ NH1 NH2  
REMARK 470 GLN A 133 CG CD OE1 NE2  
REMARK 470 GLN A 136 CG CD OE1 NE2  
REMARK 470 GLN A 137 CG CD OE1 NE2  
REMARK 470 ARG A 156 CG CD NE CZ NH1 NH2  
REMARK 470 LYS A 157 CD CE NZ  
REMARK 470 LYS A 311 CG CD CE NZ  
REMARK 500  
REMARK 500 GEOMETRY AND STEREOCHEMISTRY  
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES  
REMARK 500  
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES  
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE  
REMARK 500 THAN 6\*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN  
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).  
REMARK 500  
REMARK 500 STANDARD TABLE:  
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3 (1X, A4, 2X), 12X, F5.1)  
REMARK 500  
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991  
REMARK 500  
REMARK 500 M RES CSSEQI ATM1 ATM2 ATM3  
REMARK 500 TYR A 261 N - CA - C ANGL. DEV. = -10.1 DEGREES  
REMARK 500  
REMARK 500 REMARK: NULL  
REMARK 500

REMARK 500 GEOMETRY AND STEREOCHEMISTRY  
 REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS  
 REMARK 500  
 REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES  
 REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE  
 REMARK 500 THAN 6\*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL  
 REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE  
 REMARK 500 NUMBER; I=INSERTION CODE).  
 REMARK 500  
 REMARK 500 STANDARD TABLE:  
 REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,1X,2(A4,A1,3X),12X,F5.3)  
 REMARK 500  
 REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991  
 REMARK 500  

| M | RES | CSSEQI | ATM1 | RES | CSSEQI | ATM2 | DEVIATION |    |        |
|---|-----|--------|------|-----|--------|------|-----------|----|--------|
|   | MET | A      | 343  | SD  | MET    | A    | 343       | CE | -0.151 |

 REMARK 500  
 REMARK 500 REMARK: NULL  
 REMARK 500  
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY  
 REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT  
 REMARK 500  
 REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.  
 REMARK 500  

| ATM1 | RES | C | SSEQI | ATM2 | RES | C | SSEQI | DISTANCE |
|------|-----|---|-------|------|-----|---|-------|----------|
| OG1  | THR | A | 39    | OE1  | GLU | A | 262   | 2.16     |

 REMARK 500  
 REMARK 525  
 REMARK 525 SOLVENT  
 REMARK 525  
 REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO  
 REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY  
 REMARK 525 ASSOCIATED WITH:  

| PROTEIN CHAIN | SOLVENT CHAIN |
|---------------|---------------|
| A             | Z             |

 REMARK 525  
 REMARK 600  
 REMARK 600 HETEROGEN  
 REMARK 600  
 REMARK 600 FOR METAL ATOM FE FE2 A1350 THE COORDINATION ANGLES ARE:  

|              | 1     | 2     | 3    | 4    |
|--------------|-------|-------|------|------|
| HIS 199A NE2 |       |       |      |      |
| ASP 201A OD2 | 106.1 |       |      |      |
| HIS 279A NE2 | 77.8  | 85.5  |      |      |
| AKG 1351A O1 | 168.0 | 81.1  | 93.4 |      |
| AKG 1351A O5 | 88.7  | 163.3 | 90.2 | 83.1 |

 REMARK 600  
 REMARK 700  
 REMARK 700 SHEET  
 REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN  
 REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,  
 REMARK 700 TWO SHEETS ARE DEFINED.  
 REMARK 800  
 REMARK 800 SITE  
 REMARK 800 SITE\_IDENTIFIER: FEA  
 REMARK 800 SITE\_DESCRIPTION: FE BINDING SITE FOR CHAIN A  
 REMARK 800  
 REMARK 800 SITE\_IDENTIFIER: AKG  
 REMARK 800 SITE\_DESCRIPTION: AKG BINDING SITE FOR CHAIN A  
 REMARK 800  
 REMARK 800 SITE\_IDENTIFIER: SA1  
 REMARK 800 SITE\_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A  
 REMARK 800



REMARK 800 SITE\_IDENTIFIER: SA2  
 REMARK 800 SITE\_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A  
 REMARK 800  
 REMARK 800 SITE\_IDENTIFIER: SA3  
 REMARK 800 SITE\_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A  
 REMARK 900  
 REMARK 900 RELATED ENTRIES  
 REMARK 900 RELATED ID: 1H2K RELATED DB: PDB  
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX  
 REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE  
 REMARK 900 RELATED ID: 1H2L RELATED DB: PDB  
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX  
 REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE  
 REMARK 900 RELATED ID: 1H2M RELATED DB: PDB  
 REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX  
 REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE  
 DBREF 1H2N A 1 349 SWS Q969Q7 Q969Q7 1 349  
 SEQRES 1 A 349 MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER  
 SEQRES 2 A 349 GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA  
 SEQRES 3 A 349 TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR  
 SEQRES 4 A 349 ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA  
 SEQRES 5 A 349 GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR  
 SEQRES 6 A 349 ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU  
 SEQRES 7 A 349 GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER  
 SEQRES 8 A 349 VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP  
 SEQRES 9 A 349 GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG  
 SEQRES 10 A 349 SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU  
 SEQRES 11 A 349 LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG  
 SEQRES 12 A 349 LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG  
 SEQRES 13 A 349 LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP  
 SEQRES 14 A 349 ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU  
 SEQRES 15 A 349 THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL  
 SEQRES 16 A 349 THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA  
 SEQRES 17 A 349 GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO  
 SEQRES 18 A 349 ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS  
 SEQRES 19 A 349 PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO  
 SEQRES 20 A 349 ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY  
 SEQRES 21 A 349 TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE  
 SEQRES 22 A 349 PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN  
 SEQRES 23 A 349 GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY  
 SEQRES 24 A 349 ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA  
 SEQRES 25 A 349 HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET  
 SEQRES 26 A 349 LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO  
 SEQRES 27 A 349 LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN  
 HET FE2 A1350 1  
 HET AKG A1351 10  
 HET SO4 A1352 5  
 HET SO4 A1353 5  
 HET SO4 A1354 5  
 HETNAM FE2 FE (II) ION  
 HETNAM AKG 2-OXYGLUTARIC ACID  
 HETNAM SO4 SULFATE ION  
 FORMUL 3 FE2 FE1 2+  
 FORMUL 4 AKG C5 H6 O5  
 FORMUL 5 SO4 3(O4 S1 2-)  
 FORMUL 6 HOH \*3(H2 O1)  
 HELIX 1 1 ASP A 28 LEU A 32 5  
 HELIX 2 2 ASP A 49 ASN A 58 1  
 HELIX 3 3 VAL A 70 TRP A 76 5  
 HELIX 4 4 ASP A 77 ILE A 85 1  
 HELIX 5 5 ASP A 104 GLN A 112 5

5  
 10  
 7  
 9  
 9

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|      |    |     |     |   |    |        |        |        |      |       |   |
|------|----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 11 | CG  | PRO | A | 16 | 4.749  | 30.155 | 12.612 | 1.00 | 42.41 | C |
| ATOM | 12 | CD  | PRO | A | 16 | 5.103  | 30.916 | 11.382 | 1.00 | 42.22 | C |
| ATOM | 13 | N   | ARG | A | 17 | 7.231  | 26.791 | 10.446 | 1.00 | 42.51 | N |
| ATOM | 14 | CA  | ARG | A | 17 | 7.337  | 25.723 | 9.478  | 1.00 | 42.62 | C |
| ATOM | 15 | C   | ARG | A | 17 | 6.095  | 24.856 | 9.527  | 1.00 | 42.85 | C |
| ATOM | 16 | O   | ARG | A | 17 | 5.492  | 24.705 | 10.587 | 1.00 | 43.51 | O |
| ATOM | 17 | CB  | ARG | A | 17 | 8.505  | 24.800 | 9.845  | 1.00 | 42.50 | C |
| ATOM | 18 | CG  | ARG | A | 17 | 9.871  | 25.434 | 9.859  | 1.00 | 42.22 | C |
| ATOM | 19 | CD  | ARG | A | 17 | 10.995 | 24.466 | 10.228 | 1.00 | 42.12 | C |
| ATOM | 20 | NE  | ARG | A | 17 | 11.085 | 24.138 | 11.656 | 1.00 | 42.49 | N |
| ATOM | 21 | CZ  | ARG | A | 17 | 11.588 | 24.943 | 12.607 | 1.00 | 42.43 | C |
| ATOM | 22 | NH1 | ARG | A | 17 | 12.033 | 26.158 | 12.316 | 1.00 | 42.11 | N |
| ATOM | 23 | NH2 | ARG | A | 17 | 11.649 | 24.529 | 13.869 | 1.00 | 42.25 | N |
| ATOM | 24 | N   | GLU | A | 18 | 5.742  | 24.242 | 8.404  | 1.00 | 42.60 | N |
| ATOM | 25 | CA  | GLU | A | 18 | 4.662  | 23.268 | 8.405  | 1.00 | 42.36 | C |
| ATOM | 26 | C   | GLU | A | 18 | 5.203  | 21.870 | 8.728  | 1.00 | 41.90 | C |
| ATOM | 27 | O   | GLU | A | 18 | 6.249  | 21.472 | 8.216  | 1.00 | 41.98 | O |
| ATOM | 28 | CB  | GLU | A | 18 | 3.988  | 23.224 | 7.041  | 1.00 | 42.57 | C |
| ATOM | 29 | CG  | GLU | A | 18 | 3.363  | 24.537 | 6.620  | 1.00 | 43.60 | C |
| ATOM | 30 | CD  | GLU | A | 18 | 1.993  | 24.756 | 7.233  | 1.00 | 45.11 | C |
| ATOM | 31 | OE1 | GLU | A | 18 | 1.365  | 23.766 | 7.686  | 1.00 | 45.48 | O |
| ATOM | 32 | OE2 | GLU | A | 18 | 1.546  | 25.926 | 7.253  | 1.00 | 46.49 | O |
| ATOM | 33 | N   | GLU | A | 19 | 4.487  | 21.133 | 9.578  | 1.00 | 41.27 | N |
| ATOM | 34 | CA  | GLU | A | 19 | 4.806  | 19.737 | 9.894  | 1.00 | 40.61 | C |
| ATOM | 35 | C   | GLU | A | 19 | 4.478  | 18.802 | 8.748  | 1.00 | 39.73 | C |
| ATOM | 36 | O   | GLU | A | 19 | 3.424  | 18.915 | 8.137  | 1.00 | 39.76 | O |
| ATOM | 37 | CB  | GLU | A | 19 | 4.024  | 19.299 | 11.128 | 1.00 | 40.72 | C |
| ATOM | 38 | CG  | GLU | A | 19 | 4.507  | 20.034 | 12.361 | 1.00 | 42.24 | C |
| ATOM | 39 | CD  | GLU | A | 19 | 4.358  | 19.278 | 13.668 | 1.00 | 44.37 | C |
| ATOM | 40 | OE1 | GLU | A | 19 | 3.852  | 18.127 | 13.680 | 1.00 | 46.17 | O |
| ATOM | 41 | OE2 | GLU | A | 19 | 4.769  | 19.863 | 14.700 | 1.00 | 45.44 | O |
| ATOM | 42 | N   | ALA | A | 20 | 5.369  | 17.859 | 8.478  | 1.00 | 38.99 | N |
| ATOM | 43 | CA  | ALA | A | 20 | 5.164  | 16.922 | 7.390  | 1.00 | 38.71 | C |
| ATOM | 44 | C   | ALA | A | 20 | 3.831  | 16.232 | 7.542  | 1.00 | 38.51 | C |
| ATOM | 45 | O   | ALA | A | 20 | 3.391  | 15.933 | 8.649  | 1.00 | 38.80 | O |
| ATOM | 46 | CB  | ALA | A | 20 | 6.280  | 15.895 | 7.328  | 1.00 | 38.51 | C |
| ATOM | 47 | N   | GLY | A | 21 | 3.180  | 15.991 | 6.419  | 1.00 | 38.03 | N |
| ATOM | 48 | CA  | GLY | A | 21 | 1.924  | 15.290 | 6.449  | 1.00 | 38.11 | C |
| ATOM | 49 | C   | GLY | A | 21 | 0.746  | 16.205 | 6.682  | 1.00 | 38.19 | C |
| ATOM | 50 | O   | GLY | A | 21 | -0.328 | 15.743 | 7.049  | 1.00 | 38.25 | O |
| ATOM | 51 | N   | ALA | A | 22 | 0.941  | 17.497 | 6.447  | 1.00 | 38.40 | N |
| ATOM | 52 | CA  | ALA | A | 22 | -0.130 | 18.472 | 6.571  | 1.00 | 38.50 | C |
| ATOM | 53 | C   | ALA | A | 22 | -0.725 | 18.413 | 7.960  | 1.00 | 38.60 | C |
| ATOM | 54 | O   | ALA | A | 22 | -1.930 | 18.547 | 8.142  | 1.00 | 38.65 | O |
| ATOM | 55 | CB  | ALA | A | 22 | -1.196 | 18.242 | 5.520  | 1.00 | 38.61 | C |
| ATOM | 56 | N   | LEU | A | 23 | 0.135  | 18.206 | 8.946  | 1.00 | 38.75 | N |
| ATOM | 57 | CA  | LEU | A | 23 | -0.297 | 18.257 | 10.330 | 1.00 | 38.82 | C |
| ATOM | 58 | C   | LEU | A | 23 | -0.321 | 19.684 | 10.843 | 1.00 | 38.78 | C |
| ATOM | 59 | O   | LEU | A | 23 | -0.525 | 19.919 | 12.030 | 1.00 | 38.74 | O |
| ATOM | 60 | CB  | LEU | A | 23 | 0.597  | 17.392 | 11.193 | 1.00 | 38.77 | C |
| ATOM | 61 | CG  | LEU | A | 23 | 0.421  | 15.952 | 10.736 | 1.00 | 39.03 | C |
| ATOM | 62 | CD1 | LEU | A | 23 | 1.203  | 14.958 | 11.579 | 1.00 | 39.08 | C |
| ATOM | 63 | CD2 | LEU | A | 23 | -1.070 | 15.636 | 10.750 | 1.00 | 39.43 | C |
| ATOM | 64 | N   | GLY | A | 24 | -0.094 | 20.636 | 9.947  | 1.00 | 38.75 | N |
| ATOM | 65 | CA  | GLY | A | 24 | -0.248 | 22.025 | 10.298 | 1.00 | 38.79 | C |
| ATOM | 66 | C   | GLY | A | 24 | 0.972  | 22.669 | 10.861 | 1.00 | 38.90 | C |
| ATOM | 67 | O   | GLY | A | 24 | 2.042  | 22.084 | 10.961 | 1.00 | 39.06 | O |
| ATOM | 68 | N   | PRO | A | 25 | 0.791  | 23.906 | 11.267 | 1.00 | 39.19 | N |
| ATOM | 69 | CA  | PRO | A | 25 | 1.903  | 24.682 | 11.778 | 1.00 | 39.35 | C |
| ATOM | 70 | C   | PRO | A | 25 | 2.332  | 24.037 | 13.074 | 1.00 | 39.62 | C |
| ATOM | 71 | O   | PRO | A | 25 | 1.492  | 23.633 | 13.871 | 1.00 | 39.48 | O |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 72  | CB  | PRO | A | 25 | 1.299  | 26.062 | 12.019 | 1.00 | 39.24 | C |
| ATOM | 73  | CG  | PRO | A | 25 | -0.142 | 25.920 | 11.961 | 1.00 | 38.71 | C |
| ATOM | 74  | CD  | PRO | A | 25 | -0.490 | 24.616 | 11.365 | 1.00 | 39.17 | C |
| ATOM | 75  | N   | ALA | A | 26 | 3.631  | 23.899 | 13.252 | 1.00 | 40.22 | N |
| ATOM | 76  | CA  | ALA | A | 26 | 4.170  | 23.342 | 14.476 | 1.00 | 40.79 | C |
| ATOM | 77  | C   | ALA | A | 26 | 3.930  | 24.294 | 15.666 | 1.00 | 41.07 | C |
| ATOM | 78  | O   | ALA | A | 26 | 3.769  | 23.837 | 16.797 | 1.00 | 41.57 | O |
| ATOM | 79  | CB  | ALA | A | 26 | 5.633  | 23.068 | 14.300 | 1.00 | 40.98 | C |
| ATOM | 80  | N   | TRP | A | 27 | 3.931  | 25.605 | 15.429 | 1.00 | 40.80 | N |
| ATOM | 81  | CA  | TRP | A | 27 | 3.543  | 26.552 | 16.477 | 1.00 | 40.67 | C |
| ATOM | 82  | C   | TRP | A | 27 | 2.982  | 27.848 | 15.880 | 1.00 | 40.33 | C |
| ATOM | 83  | O   | TRP | A | 27 | 2.777  | 27.940 | 14.675 | 1.00 | 40.13 | O |
| ATOM | 84  | CB  | TRP | A | 27 | 4.742  | 26.860 | 17.358 | 1.00 | 40.70 | C |
| ATOM | 85  | CG  | TRP | A | 27 | 5.942  | 27.014 | 16.558 | 1.00 | 41.36 | C |
| ATOM | 86  | CD1 | TRP | A | 27 | 6.762  | 26.023 | 16.074 | 1.00 | 43.03 | C |
| ATOM | 87  | CD2 | TRP | A | 27 | 6.466  | 28.233 | 16.084 | 1.00 | 40.41 | C |
| ATOM | 88  | NE1 | TRP | A | 27 | 7.788  | 26.579 | 15.344 | 1.00 | 42.65 | N |
| ATOM | 89  | CE2 | TRP | A | 27 | 7.618  | 27.938 | 15.331 | 1.00 | 41.20 | C |
| ATOM | 90  | CE3 | TRP | A | 27 | 6.081  | 29.555 | 16.223 | 1.00 | 40.47 | C |
| ATOM | 91  | CZ2 | TRP | A | 27 | 8.370  | 28.912 | 14.732 | 1.00 | 41.10 | C |
| ATOM | 92  | CZ3 | TRP | A | 27 | 6.827  | 30.514 | 15.640 | 1.00 | 41.11 | C |
| ATOM | 93  | CH2 | TRP | A | 27 | 7.962  | 30.198 | 14.900 | 1.00 | 41.57 | C |
| ATOM | 94  | N   | ASP | A | 28 | 2.677  | 28.830 | 16.723 | 1.00 | 39.99 | N |
| ATOM | 95  | CA  | ASP | A | 28 | 2.322  | 30.143 | 16.209 | 1.00 | 39.78 | C |
| ATOM | 96  | C   | ASP | A | 28 | 2.802  | 31.257 | 17.121 | 1.00 | 39.17 | C |
| ATOM | 97  | O   | ASP | A | 28 | 3.227  | 31.013 | 18.240 | 1.00 | 39.00 | O |
| ATOM | 98  | CB  | ASP | A | 28 | 0.826  | 30.254 | 15.981 | 1.00 | 40.16 | C |
| ATOM | 99  | CG  | ASP | A | 28 | 0.066  | 30.380 | 17.258 | 1.00 | 40.79 | C |
| ATOM | 100 | OD1 | ASP | A | 28 | 0.044  | 31.496 | 17.821 | 1.00 | 41.30 | O |
| ATOM | 101 | OD2 | ASP | A | 28 | -0.531 | 29.414 | 17.774 | 1.00 | 42.25 | O |
| ATOM | 102 | N   | GLU | A | 29 | 2.720  | 32.486 | 16.624 | 1.00 | 38.73 | N |
| ATOM | 103 | CA  | GLU | A | 29 | 3.223  | 33.663 | 17.341 | 1.00 | 38.23 | C |
| ATOM | 104 | C   | GLU | A | 29 | 2.739  | 33.764 | 18.781 | 1.00 | 37.69 | C |
| ATOM | 105 | O   | GLU | A | 29 | 3.492  | 34.131 | 19.664 | 1.00 | 37.34 | O |
| ATOM | 106 | CB  | GLU | A | 29 | 2.834  | 34.924 | 16.594 | 1.00 | 38.20 | C |
| ATOM | 107 | N   | SER | A | 30 | 1.482  | 33.418 | 19.012 | 1.00 | 37.46 | N |
| ATOM | 108 | CA  | SER | A | 30 | 0.874  | 33.583 | 20.324 | 1.00 | 37.18 | C |
| ATOM | 109 | C   | SER | A | 30 | 1.562  | 32.774 | 21.399 | 1.00 | 36.93 | C |
| ATOM | 110 | O   | SER | A | 30 | 1.282  | 32.949 | 22.577 | 1.00 | 36.82 | O |
| ATOM | 111 | CB  | SER | A | 30 | -0.595 | 33.164 | 20.284 | 1.00 | 37.23 | C |
| ATOM | 112 | OG  | SER | A | 30 | -0.744 | 31.792 | 20.619 | 1.00 | 36.97 | O |
| ATOM | 113 | N   | GLN | A | 31 | 2.441  | 31.867 | 20.999 | 1.00 | 36.85 | N |
| ATOM | 114 | CA  | GLN | A | 31 | 3.128  | 31.021 | 21.961 | 1.00 | 36.77 | C |
| ATOM | 115 | C   | GLN | A | 31 | 4.445  | 31.636 | 22.340 | 1.00 | 36.59 | C |
| ATOM | 116 | O   | GLN | A | 31 | 5.141  | 31.127 | 23.220 | 1.00 | 36.74 | O |
| ATOM | 117 | CB  | GLN | A | 31 | 3.366  | 29.621 | 21.395 | 1.00 | 36.71 | C |
| ATOM | 118 | CG  | GLN | A | 31 | 2.084  | 28.828 | 21.234 | 1.00 | 36.97 | C |
| ATOM | 119 | CD  | GLN | A | 31 | 2.282  | 27.497 | 20.560 | 1.00 | 36.68 | C |
| ATOM | 120 | OE1 | GLN | A | 31 | 2.133  | 27.386 | 19.346 | 1.00 | 36.62 | O |
| ATOM | 121 | NE2 | GLN | A | 31 | 2.601  | 26.478 | 21.343 | 1.00 | 36.85 | N |
| ATOM | 122 | N   | LEU | A | 32 | 4.794  | 32.726 | 21.670 | 1.00 | 36.32 | N |
| ATOM | 123 | CA  | LEU | A | 32 | 6.050  | 33.381 | 21.942 | 1.00 | 36.17 | C |
| ATOM | 124 | C   | LEU | A | 32 | 5.817  | 34.498 | 22.921 | 1.00 | 36.09 | C |
| ATOM | 125 | O   | LEU | A | 32 | 4.837  | 35.233 | 22.815 | 1.00 | 36.18 | O |
| ATOM | 126 | CB  | LEU | A | 32 | 6.673  | 33.928 | 20.664 | 1.00 | 36.07 | C |
| ATOM | 127 | CG  | LEU | A | 32 | 6.990  | 32.871 | 19.604 | 1.00 | 36.72 | C |
| ATOM | 128 | CD1 | LEU | A | 32 | 7.747  | 33.457 | 18.453 | 1.00 | 36.96 | C |
| ATOM | 129 | CD2 | LEU | A | 32 | 7.797  | 31.744 | 20.161 | 1.00 | 37.31 | C |
| ATOM | 130 | N   | ARG | A | 33 | 6.700  | 34.576 | 23.908 | 1.00 | 35.99 | N |
| ATOM | 131 | CA  | ARG | A | 33 | 6.713  | 35.671 | 24.851 | 1.00 | 36.15 | C |
| ATOM | 132 | C   | ARG | A | 33 | 7.171  | 36.941 | 24.130 | 1.00 | 35.95 | C |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 133 | O   | ARG | A | 33 | 7.950  | 36.888 | 23.188 | 1.00 | 35.75 | O |
| ATOM | 134 | CB  | ARG | A | 33 | 7.671  | 35.350 | 25.991 | 1.00 | 36.41 | C |
| ATOM | 135 | CG  | ARG | A | 33 | 7.210  | 34.204 | 26.854 | 1.00 | 36.76 | C |
| ATOM | 136 | CD  | ARG | A | 33 | 8.082  | 33.948 | 28.070 | 1.00 | 36.81 | C |
| ATOM | 137 | NE  | ARG | A | 33 | 7.479  | 32.927 | 28.923 | 1.00 | 37.39 | N |
| ATOM | 138 | CZ  | ARG | A | 33 | 6.501  | 33.160 | 29.785 | 1.00 | 37.61 | C |
| ATOM | 139 | NH1 | ARG | A | 33 | 6.027  | 34.385 | 29.931 | 1.00 | 37.75 | N |
| ATOM | 140 | NH2 | ARG | A | 33 | 6.001  | 32.171 | 30.513 | 1.00 | 38.47 | N |
| ATOM | 141 | N   | SER | A | 34 | 6.707  | 38.088 | 24.588 | 1.00 | 35.92 | N |
| ATOM | 142 | CA  | SER | A | 34 | 7.017  | 39.331 | 23.902 | 1.00 | 36.05 | C |
| ATOM | 143 | C   | SER | A | 34 | 8.044  | 40.146 | 24.671 | 1.00 | 35.47 | C |
| ATOM | 144 | O   | SER | A | 34 | 7.940  | 40.311 | 25.884 | 1.00 | 35.41 | O |
| ATOM | 145 | CB  | SER | A | 34 | 5.732  | 40.120 | 23.691 | 1.00 | 36.27 | C |
| ATOM | 146 | OG  | SER | A | 34 | 5.046  | 40.253 | 24.920 | 1.00 | 37.99 | O |
| ATOM | 147 | N   | TYR | A | 35 | 9.031  | 40.655 | 23.945 | 1.00 | 35.01 | N |
| ATOM | 148 | CA  | TYR | A | 35 | 10.140 | 41.370 | 24.543 | 1.00 | 34.69 | C |
| ATOM | 149 | C   | TYR | A | 35 | 10.400 | 42.693 | 23.853 | 1.00 | 34.59 | C |
| ATOM | 150 | O   | TYR | A | 35 | 9.841  | 42.989 | 22.813 | 1.00 | 34.45 | O |
| ATOM | 151 | CB  | TYR | A | 35 | 11.384 | 40.501 | 24.469 | 1.00 | 34.71 | C |
| ATOM | 152 | CG  | TYR | A | 35 | 11.228 | 39.222 | 25.232 | 1.00 | 34.43 | C |
| ATOM | 153 | CD1 | TYR | A | 35 | 10.928 | 39.246 | 26.573 | 1.00 | 33.87 | C |
| ATOM | 154 | CD2 | TYR | A | 35 | 11.350 | 37.986 | 24.602 | 1.00 | 35.32 | C |
| ATOM | 155 | CE1 | TYR | A | 35 | 10.775 | 38.087 | 27.285 | 1.00 | 34.96 | C |
| ATOM | 156 | CE2 | TYR | A | 35 | 11.192 | 36.807 | 25.309 | 1.00 | 35.50 | C |
| ATOM | 157 | CZ  | TYR | A | 35 | 10.904 | 36.865 | 26.653 | 1.00 | 35.16 | C |
| ATOM | 158 | OH  | TYR | A | 35 | 10.742 | 35.709 | 27.376 | 1.00 | 34.77 | O |
| ATOM | 159 | N   | SER | A | 36 | 11.290 | 43.481 | 24.429 | 1.00 | 34.77 | N |
| ATOM | 160 | CA  | SER | A | 36 | 11.572 | 44.814 | 23.924 | 1.00 | 34.74 | C |
| ATOM | 161 | C   | SER | A | 36 | 12.567 | 44.926 | 22.771 | 1.00 | 34.30 | C |
| ATOM | 162 | O   | SER | A | 36 | 12.805 | 46.011 | 22.287 | 1.00 | 34.23 | O |
| ATOM | 163 | CB  | SER | A | 36 | 12.127 | 45.627 | 25.077 | 1.00 | 34.91 | C |
| ATOM | 164 | OG  | SER | A | 36 | 13.395 | 45.116 | 25.449 | 1.00 | 35.56 | O |
| ATOM | 165 | N   | PHE | A | 37 | 13.155 | 43.838 | 22.318 | 1.00 | 34.15 | N |
| ATOM | 166 | CA  | PHE | A | 37 | 14.193 | 43.963 | 21.306 | 1.00 | 34.11 | C |
| ATOM | 167 | C   | PHE | A | 37 | 13.969 | 43.177 | 20.044 | 1.00 | 34.07 | C |
| ATOM | 168 | O   | PHE | A | 37 | 13.356 | 42.109 | 20.017 | 1.00 | 33.98 | O |
| ATOM | 169 | CB  | PHE | A | 37 | 15.514 | 43.479 | 21.867 | 1.00 | 34.08 | C |
| ATOM | 170 | CG  | PHE | A | 37 | 15.417 | 42.147 | 22.438 | 1.00 | 34.33 | C |
| ATOM | 171 | CD1 | PHE | A | 37 | 15.445 | 41.034 | 21.621 | 1.00 | 35.66 | C |
| ATOM | 172 | CD2 | PHE | A | 37 | 15.208 | 41.990 | 23.777 | 1.00 | 35.42 | C |
| ATOM | 173 | CE1 | PHE | A | 37 | 15.320 | 39.782 | 22.143 | 1.00 | 35.73 | C |
| ATOM | 174 | CE2 | PHE | A | 37 | 15.084 | 40.736 | 24.317 | 1.00 | 36.14 | C |
| ATOM | 175 | CZ  | PHE | A | 37 | 15.141 | 39.628 | 23.497 | 1.00 | 36.55 | C |
| ATOM | 176 | N   | PRO | A | 38 | 14.565 | 43.682 | 18.991 | 1.00 | 33.95 | N |
| ATOM | 177 | CA  | PRO | A | 38 | 14.474 | 43.028 | 17.704 | 1.00 | 33.91 | C |
| ATOM | 178 | C   | PRO | A | 38 | 15.445 | 41.878 | 17.640 | 1.00 | 33.74 | C |
| ATOM | 179 | O   | PRO | A | 38 | 16.366 | 41.803 | 18.441 | 1.00 | 33.82 | O |
| ATOM | 180 | CB  | PRO | A | 38 | 14.887 | 44.133 | 16.751 | 1.00 | 34.03 | C |
| ATOM | 181 | CG  | PRO | A | 38 | 15.874 | 44.935 | 17.548 | 1.00 | 33.99 | C |
| ATOM | 182 | CD  | PRO | A | 38 | 15.385 | 44.903 | 18.945 | 1.00 | 33.80 | C |
| ATOM | 183 | N   | THR | A | 39 | 15.233 | 40.996 | 16.678 | 1.00 | 34.02 | N |
| ATOM | 184 | CA  | THR | A | 39 | 16.089 | 39.844 | 16.464 | 1.00 | 34.00 | C |
| ATOM | 185 | C   | THR | A | 39 | 16.035 | 39.490 | 15.008 | 1.00 | 34.09 | C |
| ATOM | 186 | O   | THR | A | 39 | 15.137 | 39.894 | 14.311 | 1.00 | 34.05 | O |
| ATOM | 187 | CB  | THR | A | 39 | 15.563 | 38.637 | 17.201 | 1.00 | 33.94 | C |
| ATOM | 188 | OG1 | THR | A | 39 | 14.250 | 38.336 | 16.714 | 1.00 | 34.18 | O |
| ATOM | 189 | CG2 | THR | A | 39 | 15.338 | 38.915 | 18.642 | 1.00 | 34.09 | C |
| ATOM | 190 | N   | ARG | A | 40 | 16.992 | 38.695 | 14.576 | 1.00 | 34.62 | N |
| ATOM | 191 | CA  | ARG | A | 40 | 17.066 | 38.204 | 13.228 | 1.00 | 35.13 | C |
| ATOM | 192 | C   | ARG | A | 40 | 17.100 | 36.721 | 13.361 | 1.00 | 35.17 | C |
| ATOM | 193 | O   | ARG | A | 40 | 17.419 | 36.189 | 14.434 | 1.00 | 34.96 | O |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 194 | CB  | ARG | A | 40 | 18.352 | 38.649 | 12.568 | 1.00 | 35.54 | C |
| ATOM | 195 | CG  | ARG | A | 40 | 18.358 | 40.103 | 12.287 | 1.00 | 38.87 | C |
| ATOM | 196 | CD  | ARG | A | 40 | 16.975 | 40.597 | 11.893 | 1.00 | 42.88 | C |
| ATOM | 197 | NE  | ARG | A | 40 | 16.737 | 40.908 | 10.489 | 1.00 | 44.50 | N |
| ATOM | 198 | CZ  | ARG | A | 40 | 15.554 | 41.298 | 10.076 | 1.00 | 46.73 | C |
| ATOM | 199 | NH1 | ARG | A | 40 | 14.574 | 41.350 | 10.974 | 1.00 | 46.73 | N |
| ATOM | 200 | NH2 | ARG | A | 40 | 15.334 | 41.636 | 8.802  | 1.00 | 48.87 | N |
| ATOM | 201 | N   | PRO | A | 41 | 16.775 | 36.026 | 12.285 | 1.00 | 35.20 | N |
| ATOM | 202 | CA  | PRO | A | 41 | 16.749 | 34.579 | 12.348 | 1.00 | 35.24 | C |
| ATOM | 203 | C   | PRO | A | 41 | 18.114 | 33.973 | 12.275 | 1.00 | 35.10 | C |
| ATOM | 204 | O   | PRO | A | 41 | 18.995 | 34.455 | 11.573 | 1.00 | 35.96 | O |
| ATOM | 205 | CB  | PRO | A | 41 | 16.003 | 34.208 | 11.079 | 1.00 | 35.27 | C |
| ATOM | 206 | CG  | PRO | A | 41 | 15.408 | 35.453 | 10.640 | 1.00 | 34.93 | C |
| ATOM | 207 | CD  | PRO | A | 41 | 16.381 | 36.494 | 10.953 | 1.00 | 34.81 | C |
| ATOM | 208 | N   | ILE | A | 42 | 18.277 | 32.910 | 13.022 | 1.00 | 34.55 | N |
| ATOM | 209 | CA  | ILE | A | 42 | 19.435 | 32.099 | 12.909 | 1.00 | 34.29 | C |
| ATOM | 210 | C   | ILE | A | 42 | 19.145 | 31.194 | 11.713 | 1.00 | 34.29 | C |
| ATOM | 211 | O   | ILE | A | 42 | 18.035 | 30.654 | 11.598 | 1.00 | 34.38 | O |
| ATOM | 212 | CB  | ILE | A | 42 | 19.545 | 31.258 | 14.150 | 1.00 | 34.14 | C |
| ATOM | 213 | CG1 | ILE | A | 42 | 19.742 | 32.152 | 15.368 | 1.00 | 34.83 | C |
| ATOM | 214 | CG2 | ILE | A | 42 | 20.679 | 30.297 | 14.016 | 1.00 | 34.41 | C |
| ATOM | 215 | CD1 | ILE | A | 42 | 19.479 | 31.467 | 16.678 | 1.00 | 35.37 | C |
| ATOM | 216 | N   | PRO | A | 43 | 20.127 | 31.010 | 10.836 | 1.00 | 33.80 | N |
| ATOM | 217 | CA  | PRO | A | 43 | 19.982 | 30.122 | 9.686  | 1.00 | 33.62 | C |
| ATOM | 218 | C   | PRO | A | 43 | 19.714 | 28.676 | 10.066 | 1.00 | 33.65 | C |
| ATOM | 219 | O   | PRO | A | 43 | 20.320 | 28.198 | 11.015 | 1.00 | 33.60 | O |
| ATOM | 220 | CB  | PRO | A | 43 | 21.366 | 30.174 | 9.043  | 1.00 | 33.63 | C |
| ATOM | 221 | CG  | PRO | A | 43 | 21.986 | 31.385 | 9.543  | 1.00 | 33.11 | C |
| ATOM | 222 | CD  | PRO | A | 43 | 21.455 | 31.630 | 10.882 | 1.00 | 33.51 | C |
| ATOM | 223 | N   | ARG | A | 44 | 18.820 | 28.007 | 9.341  | 1.00 | 33.86 | N |
| ATOM | 224 | CA  | ARG | A | 44 | 18.597 | 26.572 | 9.486  | 1.00 | 34.00 | C |
| ATOM | 225 | C   | ARG | A | 44 | 19.176 | 25.968 | 8.247  | 1.00 | 33.87 | C |
| ATOM | 226 | O   | ARG | A | 44 | 18.783 | 26.319 | 7.152  | 1.00 | 33.76 | O |
| ATOM | 227 | CB  | ARG | A | 44 | 17.125 | 26.185 | 9.520  | 1.00 | 34.10 | C |
| ATOM | 228 | CG  | ARG | A | 44 | 16.301 | 26.879 | 10.577 | 1.00 | 35.44 | C |
| ATOM | 229 | CD  | ARG | A | 44 | 14.781 | 26.505 | 10.583 | 1.00 | 37.36 | C |
| ATOM | 230 | NE  | ARG | A | 44 | 14.415 | 25.108 | 10.265 | 1.00 | 37.59 | N |
| ATOM | 231 | CZ  | ARG | A | 44 | 14.237 | 24.144 | 11.187 | 1.00 | 39.71 | C |
| ATOM | 232 | NH1 | ARG | A | 44 | 14.429 | 24.396 | 12.487 | 1.00 | 39.94 | N |
| ATOM | 233 | NH2 | ARG | A | 44 | 13.876 | 22.915 | 10.821 | 1.00 | 40.07 | N |
| ATOM | 234 | N   | LEU | A | 45 | 20.086 | 25.030 | 8.407  | 1.00 | 33.98 | N |
| ATOM | 235 | CA  | LEU | A | 45 | 20.747 | 24.467 | 7.269  | 1.00 | 34.15 | C |
| ATOM | 236 | C   | LEU | A | 45 | 20.950 | 22.995 | 7.389  | 1.00 | 34.37 | C |
| ATOM | 237 | O   | LEU | A | 45 | 20.901 | 22.453 | 8.486  | 1.00 | 34.52 | O |
| ATOM | 238 | CB  | LEU | A | 45 | 22.116 | 25.090 | 7.183  | 1.00 | 34.25 | C |
| ATOM | 239 | CG  | LEU | A | 45 | 22.080 | 26.576 | 6.905  | 1.00 | 34.80 | C |
| ATOM | 240 | CD1 | LEU | A | 45 | 23.454 | 27.095 | 7.177  | 1.00 | 36.05 | C |
| ATOM | 241 | CD2 | LEU | A | 45 | 21.655 | 26.837 | 5.481  | 1.00 | 34.78 | C |
| ATOM | 242 | N   | SER | A | 46 | 21.199 | 22.343 | 6.255  | 1.00 | 34.55 | N |
| ATOM | 243 | CA  | SER | A | 46 | 21.549 | 20.949 | 6.306  | 1.00 | 34.60 | C |
| ATOM | 244 | C   | SER | A | 46 | 22.985 | 20.838 | 6.681  | 1.00 | 34.89 | C |
| ATOM | 245 | O   | SER | A | 46 | 23.826 | 21.671 | 6.383  | 1.00 | 34.54 | O |
| ATOM | 246 | CB  | SER | A | 46 | 21.356 | 20.206 | 5.006  | 1.00 | 34.64 | C |
| ATOM | 247 | OG  | SER | A | 46 | 22.231 | 19.090 | 4.989  | 1.00 | 33.61 | O |
| ATOM | 248 | N   | GLN | A | 47 | 23.247 | 19.736 | 7.324  | 1.00 | 35.61 | N |
| ATOM | 249 | CA  | GLN | A | 47 | 24.539 | 19.462 | 7.866  | 1.00 | 36.10 | C |
| ATOM | 250 | C   | GLN | A | 47 | 25.565 | 19.368 | 6.746  | 1.00 | 35.96 | C |
| ATOM | 251 | O   | GLN | A | 47 | 26.754 | 19.537 | 6.969  | 1.00 | 36.13 | O |
| ATOM | 252 | CB  | GLN | A | 47 | 24.399 | 18.168 | 8.669  | 1.00 | 36.22 | C |
| ATOM | 253 | CG  | GLN | A | 47 | 25.604 | 17.340 | 8.730  | 1.00 | 37.25 | C |
| ATOM | 254 | CD  | GLN | A | 47 | 25.724 | 16.459 | 7.532  | 1.00 | 39.03 | C |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 255 | OE1 | GLN | A | 47 | 24.766 | 16.306 | 6.759  | 1.00 | 38.79 | O |
| ATOM | 256 | NE2 | GLN | A | 47 | 26.902 | 15.872 | 7.354  | 1.00 | 41.44 | N |
| ATOM | 257 | N   | SER | A | 48 | 25.088 | 19.146 | 5.531  | 1.00 | 35.87 | N |
| ATOM | 258 | CA  | SER | A | 48 | 25.958 | 18.938 | 4.391  | 1.00 | 35.90 | C |
| ATOM | 259 | C   | SER | A | 48 | 26.301 | 20.244 | 3.715  | 1.00 | 36.06 | C |
| ATOM | 260 | O   | SER | A | 48 | 27.215 | 20.334 | 2.897  | 1.00 | 35.95 | O |
| ATOM | 261 | CB  | SER | A | 48 | 25.214 | 18.073 | 3.402  | 1.00 | 35.97 | C |
| ATOM | 262 | OG  | SER | A | 48 | 23.933 | 18.635 | 3.158  | 1.00 | 36.62 | O |
| ATOM | 263 | N   | ASP | A | 49 | 25.552 | 21.266 | 4.075  | 1.00 | 36.34 | N |
| ATOM | 264 | CA  | ASP | A | 49 | 25.701 | 22.564 | 3.491  | 1.00 | 36.65 | C |
| ATOM | 265 | C   | ASP | A | 49 | 26.963 | 23.236 | 3.952  | 1.00 | 37.06 | C |
| ATOM | 266 | O   | ASP | A | 49 | 27.114 | 23.507 | 5.138  | 1.00 | 37.24 | O |
| ATOM | 267 | CB  | ASP | A | 49 | 24.545 | 23.405 | 3.953  | 1.00 | 36.80 | C |
| ATOM | 268 | CG  | ASP | A | 49 | 24.441 | 24.674 | 3.206  | 1.00 | 37.08 | C |
| ATOM | 269 | OD1 | ASP | A | 49 | 25.490 | 25.217 | 2.810  | 1.00 | 37.38 | O |
| ATOM | 270 | OD2 | ASP | A | 49 | 23.343 | 25.187 | 2.953  | 1.00 | 38.64 | O |
| ATOM | 271 | N   | PRO | A | 50 | 27.857 | 23.565 | 3.029  | 1.00 | 37.42 | N |
| ATOM | 272 | CA  | PRO | A | 50 | 29.113 | 24.196 | 3.430  | 1.00 | 37.32 | C |
| ATOM | 273 | C   | PRO | A | 50 | 28.881 | 25.413 | 4.298  | 1.00 | 37.46 | C |
| ATOM | 274 | O   | PRO | A | 50 | 29.742 | 25.727 | 5.113  | 1.00 | 37.85 | O |
| ATOM | 275 | CB  | PRO | A | 50 | 29.750 | 24.604 | 2.108  | 1.00 | 37.21 | C |
| ATOM | 276 | CG  | PRO | A | 50 | 29.134 | 23.726 | 1.086  | 1.00 | 37.39 | C |
| ATOM | 277 | CD  | PRO | A | 50 | 27.755 | 23.395 | 1.568  | 1.00 | 37.34 | C |
| ATOM | 278 | N   | ARG | A | 51 | 27.743 | 26.081 | 4.162  | 1.00 | 37.64 | N |
| ATOM | 279 | CA  | ARG | A | 51 | 27.535 | 27.301 | 4.932  | 1.00 | 38.06 | C |
| ATOM | 280 | C   | ARG | A | 51 | 27.470 | 27.000 | 6.421  | 1.00 | 38.26 | C |
| ATOM | 281 | O   | ARG | A | 51 | 27.920 | 27.798 | 7.250  | 1.00 | 38.47 | O |
| ATOM | 282 | CB  | ARG | A | 51 | 26.282 | 28.055 | 4.470  | 1.00 | 38.14 | C |
| ATOM | 283 | CG  | ARG | A | 51 | 26.418 | 28.692 | 3.059  | 1.00 | 38.89 | C |
| ATOM | 284 | CD  | ARG | A | 51 | 25.117 | 29.259 | 2.455  | 1.00 | 39.65 | C |
| ATOM | 285 | NE  | ARG | A | 51 | 24.121 | 28.211 | 2.175  | 1.00 | 41.25 | N |
| ATOM | 286 | CZ  | ARG | A | 51 | 22.798 | 28.404 | 2.078  | 1.00 | 41.86 | C |
| ATOM | 287 | NH1 | ARG | A | 51 | 22.264 | 29.605 | 2.225  | 1.00 | 43.70 | N |
| ATOM | 288 | NH2 | ARG | A | 51 | 21.994 | 27.393 | 1.818  | 1.00 | 41.90 | N |
| ATOM | 289 | N   | ALA | A | 52 | 26.936 | 25.837 | 6.770  | 1.00 | 38.26 | N |
| ATOM | 290 | CA  | ALA | A | 52 | 26.807 | 25.499 | 8.171  | 1.00 | 38.30 | C |
| ATOM | 291 | C   | ALA | A | 52 | 28.206 | 25.374 | 8.683  | 1.00 | 38.45 | C |
| ATOM | 292 | O   | ALA | A | 52 | 28.572 | 25.922 | 9.732  | 1.00 | 38.37 | O |
| ATOM | 293 | CB  | ALA | A | 52 | 26.085 | 24.208 | 8.344  | 1.00 | 38.25 | C |
| ATOM | 294 | N   | GLU | A | 53 | 29.003 | 24.665 | 7.901  | 1.00 | 38.56 | N |
| ATOM | 295 | CA  | GLU | A | 53 | 30.361 | 24.420 | 8.291  | 1.00 | 38.94 | C |
| ATOM | 296 | C   | GLU | A | 53 | 31.145 | 25.717 | 8.484  | 1.00 | 39.00 | C |
| ATOM | 297 | O   | GLU | A | 53 | 31.970 | 25.793 | 9.386  | 1.00 | 38.49 | O |
| ATOM | 298 | CB  | GLU | A | 53 | 31.060 | 23.507 | 7.314  | 1.00 | 38.91 | C |
| ATOM | 299 | CG  | GLU | A | 53 | 32.139 | 22.738 | 8.035  | 1.00 | 40.55 | C |
| ATOM | 300 | CD  | GLU | A | 53 | 31.662 | 21.403 | 8.579  | 1.00 | 42.38 | C |
| ATOM | 301 | OE1 | GLU | A | 53 | 30.475 | 21.274 | 8.957  | 1.00 | 43.42 | O |
| ATOM | 302 | OE2 | GLU | A | 53 | 32.498 | 20.478 | 8.639  | 1.00 | 44.15 | O |
| ATOM | 303 | N   | GLU | A | 54 | 30.897 | 26.737 | 7.662  | 1.00 | 39.21 | N |
| ATOM | 304 | CA  | GLU | A | 54 | 31.592 | 28.004 | 7.870  | 1.00 | 39.44 | C |
| ATOM | 305 | C   | GLU | A | 54 | 31.092 | 28.625 | 9.144  | 1.00 | 39.05 | C |
| ATOM | 306 | O   | GLU | A | 54 | 31.848 | 29.262 | 9.869  | 1.00 | 39.51 | O |
| ATOM | 307 | CB  | GLU | A | 54 | 31.337 | 29.023 | 6.772  | 1.00 | 39.59 | C |
| ATOM | 308 | CG  | GLU | A | 54 | 31.940 | 28.693 | 5.433  | 1.00 | 41.75 | C |
| ATOM | 309 | CD  | GLU | A | 54 | 31.098 | 29.263 | 4.302  | 1.00 | 44.74 | C |
| ATOM | 310 | OE1 | GLU | A | 54 | 30.546 | 30.379 | 4.509  | 1.00 | 46.67 | O |
| ATOM | 311 | OE2 | GLU | A | 54 | 30.972 | 28.596 | 3.234  | 1.00 | 44.49 | O |
| ATOM | 312 | N   | LEU | A | 55 | 29.812 | 28.468 | 9.424  | 1.00 | 38.37 | N |
| ATOM | 313 | CA  | LEU | A | 55 | 29.291 | 29.137 | 10.583 | 1.00 | 38.08 | C |
| ATOM | 314 | C   | LEU | A | 55 | 29.906 | 28.613 | 11.847 | 1.00 | 37.88 | C |
| ATOM | 315 | O   | LEU | A | 55 | 30.359 | 29.397 | 12.693 | 1.00 | 37.59 | O |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 316 | CB  | LEU | A | 55 | 27.789 | 29.006 | 10.648 | 1.00 | 38.28 | C |
| ATOM | 317 | CG  | LEU | A | 55 | 27.142 | 29.846 | 9.564  | 1.00 | 37.79 | C |
| ATOM | 318 | CD1 | LEU | A | 55 | 25.722 | 29.443 | 9.409  | 1.00 | 38.31 | C |
| ATOM | 319 | CD2 | LEU | A | 55 | 27.233 | 31.279 | 9.951  | 1.00 | 37.31 | C |
| ATOM | 320 | N   | ILE | A | 56 | 29.938 | 27.286 | 11.971 | 1.00 | 37.71 | N |
| ATOM | 321 | CA  | ILE | A | 56 | 30.455 | 26.667 | 13.183 | 1.00 | 37.35 | C |
| ATOM | 322 | C   | ILE | A | 56 | 31.912 | 26.988 | 13.321 | 1.00 | 37.30 | C |
| ATOM | 323 | O   | ILE | A | 56 | 32.373 | 27.320 | 14.406 | 1.00 | 36.89 | O |
| ATOM | 324 | CB  | ILE | A | 56 | 30.288 | 25.171 | 13.175 | 1.00 | 37.30 | C |
| ATOM | 325 | CG1 | ILE | A | 56 | 28.810 | 24.789 | 13.213 | 1.00 | 36.97 | C |
| ATOM | 326 | CG2 | ILE | A | 56 | 30.968 | 24.602 | 14.397 | 1.00 | 37.75 | C |
| ATOM | 327 | CD1 | ILE | A | 56 | 28.543 | 23.358 | 12.820 | 1.00 | 36.35 | C |
| ATOM | 328 | N   | GLU | A | 57 | 32.627 | 26.899 | 12.204 | 1.00 | 37.67 | N |
| ATOM | 329 | CA  | GLU | A | 57 | 34.045 | 27.204 | 12.166 | 1.00 | 38.21 | C |
| ATOM | 330 | C   | GLU | A | 57 | 34.277 | 28.569 | 12.784 | 1.00 | 38.33 | C |
| ATOM | 331 | O   | GLU | A | 57 | 35.210 | 28.758 | 13.566 | 1.00 | 38.33 | O |
| ATOM | 332 | CB  | GLU | A | 57 | 34.547 | 27.214 | 10.725 | 1.00 | 38.49 | C |
| ATOM | 333 | CG  | GLU | A | 57 | 36.038 | 27.461 | 10.559 | 1.00 | 40.09 | C |
| ATOM | 334 | CD  | GLU | A | 57 | 36.870 | 26.539 | 11.424 | 1.00 | 42.96 | C |
| ATOM | 335 | OE1 | GLU | A | 57 | 36.527 | 25.329 | 11.487 | 1.00 | 43.20 | O |
| ATOM | 336 | OE2 | GLU | A | 57 | 37.852 | 27.032 | 12.044 | 1.00 | 44.14 | O |
| ATOM | 337 | N   | ASN | A | 58 | 33.394 | 29.508 | 12.460 | 1.00 | 38.32 | N |
| ATOM | 338 | CA  | ASN | A | 58 | 33.546 | 30.890 | 12.891 | 1.00 | 38.38 | C |
| ATOM | 339 | C   | ASN | A | 58 | 32.849 | 31.221 | 14.167 | 1.00 | 38.06 | C |
| ATOM | 340 | O   | ASN | A | 58 | 32.683 | 32.387 | 14.507 | 1.00 | 37.86 | O |
| ATOM | 341 | CB  | ASN | A | 58 | 32.955 | 31.813 | 11.853 | 1.00 | 38.73 | C |
| ATOM | 342 | CG  | ASN | A | 58 | 33.991 | 32.455 | 11.013 | 1.00 | 39.49 | C |
| ATOM | 343 | OD1 | ASN | A | 58 | 34.501 | 31.841 | 10.083 | 1.00 | 42.51 | O |
| ATOM | 344 | ND2 | ASN | A | 58 | 34.322 | 33.704 | 11.324 | 1.00 | 40.15 | N |
| ATOM | 345 | N   | GLU | A | 59 | 32.399 | 30.196 | 14.856 | 1.00 | 37.88 | N |
| ATOM | 346 | CA  | GLU | A | 59 | 31.683 | 30.396 | 16.092 | 1.00 | 37.68 | C |
| ATOM | 347 | C   | GLU | A | 59 | 30.479 | 31.307 | 16.005 | 1.00 | 37.57 | C |
| ATOM | 348 | O   | GLU | A | 59 | 30.305 | 32.203 | 16.813 | 1.00 | 36.94 | O |
| ATOM | 349 | CB  | GLU | A | 59 | 32.663 | 30.857 | 17.118 | 1.00 | 37.60 | C |
| ATOM | 350 | CG  | GLU | A | 59 | 33.710 | 29.785 | 17.212 | 1.00 | 38.25 | C |
| ATOM | 351 | CD  | GLU | A | 59 | 34.545 | 29.886 | 18.435 | 1.00 | 38.10 | C |
| ATOM | 352 | OE1 | GLU | A | 59 | 35.654 | 30.430 | 18.303 | 1.00 | 40.30 | O |
| ATOM | 353 | OE2 | GLU | A | 59 | 34.089 | 29.420 | 19.498 | 1.00 | 37.62 | O |
| ATOM | 354 | N   | GLU | A | 60 | 29.630 | 31.025 | 15.025 | 1.00 | 37.73 | N |
| ATOM | 355 | CA  | GLU | A | 60 | 28.347 | 31.692 | 14.902 | 1.00 | 37.79 | C |
| ATOM | 356 | C   | GLU | A | 60 | 27.290 | 30.620 | 14.923 | 1.00 | 37.12 | C |
| ATOM | 357 | O   | GLU | A | 60 | 27.488 | 29.539 | 14.388 | 1.00 | 37.94 | O |
| ATOM | 358 | CB  | GLU | A | 60 | 28.252 | 32.456 | 13.606 | 1.00 | 38.14 | C |
| ATOM | 359 | CG  | GLU | A | 60 | 29.388 | 33.411 | 13.414 | 1.00 | 39.56 | C |
| ATOM | 360 | CD  | GLU | A | 60 | 28.986 | 34.547 | 12.518 | 1.00 | 42.62 | C |
| ATOM | 361 | OE1 | GLU | A | 60 | 29.023 | 34.389 | 11.276 | 1.00 | 42.22 | O |
| ATOM | 362 | OE2 | GLU | A | 60 | 28.611 | 35.601 | 13.082 | 1.00 | 46.90 | O |
| ATOM | 363 | N   | PRO | A | 61 | 26.158 | 30.917 | 15.517 | 1.00 | 36.25 | N |
| ATOM | 364 | CA  | PRO | A | 61 | 25.111 | 29.919 | 15.680 | 1.00 | 36.11 | C |
| ATOM | 365 | C   | PRO | A | 61 | 24.522 | 29.448 | 14.373 | 1.00 | 35.80 | C |
| ATOM | 366 | O   | PRO | A | 61 | 24.534 | 30.159 | 13.386 | 1.00 | 36.29 | O |
| ATOM | 367 | CB  | PRO | A | 61 | 24.021 | 30.672 | 16.442 | 1.00 | 36.35 | C |
| ATOM | 368 | CG  | PRO | A | 61 | 24.367 | 32.117 | 16.353 | 1.00 | 36.05 | C |
| ATOM | 369 | CD  | PRO | A | 61 | 25.790 | 32.228 | 16.061 | 1.00 | 36.10 | C |
| ATOM | 370 | N   | VAL | A | 62 | 23.981 | 28.247 | 14.380 | 1.00 | 35.41 | N |
| ATOM | 371 | CA  | VAL | A | 62 | 23.291 | 27.722 | 13.228 | 1.00 | 34.88 | C |
| ATOM | 372 | C   | VAL | A | 62 | 22.438 | 26.584 | 13.720 | 1.00 | 34.68 | C |
| ATOM | 373 | O   | VAL | A | 62 | 22.807 | 25.885 | 14.658 | 1.00 | 34.41 | O |
| ATOM | 374 | CB  | VAL | A | 62 | 24.237 | 27.189 | 12.156 | 1.00 | 34.79 | C |
| ATOM | 375 | CG1 | VAL | A | 62 | 25.108 | 26.062 | 12.695 | 1.00 | 34.66 | C |
| ATOM | 376 | CG2 | VAL | A | 62 | 23.440 | 26.693 | 10.996 | 1.00 | 34.83 | C |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 377 | N   | VAL | A | 63 | 21.271 | 26.418 | 13.118 | 1.00 | 34.54 | N |
| ATOM | 378 | CA  | VAL | A | 63 | 20.454 | 25.273 | 13.447 | 1.00 | 34.18 | C |
| ATOM | 379 | C   | VAL | A | 63 | 20.660 | 24.230 | 12.372 | 1.00 | 33.85 | C |
| ATOM | 380 | O   | VAL | A | 63 | 20.486 | 24.512 | 11.203 | 1.00 | 33.36 | O |
| ATOM | 381 | CB  | VAL | A | 63 | 18.980 | 25.622 | 13.523 | 1.00 | 34.05 | C |
| ATOM | 382 | CG1 | VAL | A | 63 | 18.167 | 24.349 | 13.626 | 1.00 | 34.14 | C |
| ATOM | 383 | CG2 | VAL | A | 63 | 18.717 | 26.502 | 14.710 | 1.00 | 33.51 | C |
| ATOM | 384 | N   | LEU | A | 64 | 21.048 | 23.028 | 12.769 | 1.00 | 33.87 | N |
| ATOM | 385 | CA  | LEU | A | 64 | 21.204 | 21.942 | 11.814 | 1.00 | 34.03 | C |
| ATOM | 386 | C   | LEU | A | 64 | 19.894 | 21.193 | 11.856 | 1.00 | 33.70 | C |
| ATOM | 387 | O   | LEU | A | 64 | 19.368 | 20.956 | 12.932 | 1.00 | 34.18 | O |
| ATOM | 388 | CB  | LEU | A | 64 | 22.417 | 21.071 | 12.164 | 1.00 | 33.90 | C |
| ATOM | 389 | CG  | LEU | A | 64 | 23.667 | 21.978 | 12.155 | 1.00 | 34.85 | C |
| ATOM | 390 | CD1 | LEU | A | 64 | 24.975 | 21.303 | 12.485 | 1.00 | 35.82 | C |
| ATOM | 391 | CD2 | LEU | A | 64 | 23.821 | 22.629 | 10.798 | 1.00 | 35.39 | C |
| ATOM | 392 | N   | THR | A | 65 | 19.314 | 20.887 | 10.704 | 1.00 | 33.36 | N |
| ATOM | 393 | CA  | THR | A | 65 | 18.035 | 20.177 | 10.704 | 1.00 | 33.24 | C |
| ATOM | 394 | C   | THR | A | 65 | 18.105 | 18.683 | 10.517 | 1.00 | 32.87 | C |
| ATOM | 395 | O   | THR | A | 65 | 17.096 | 18.016 | 10.715 | 1.00 | 32.11 | O |
| ATOM | 396 | CB  | THR | A | 65 | 17.149 | 20.657 | 9.562  | 1.00 | 33.35 | C |
| ATOM | 397 | OG1 | THR | A | 65 | 17.858 | 20.540 | 8.320  | 1.00 | 33.15 | O |
| ATOM | 398 | CG2 | THR | A | 65 | 16.843 | 22.093 | 9.693  | 1.00 | 33.51 | C |
| ATOM | 399 | N   | ASP | A | 66 | 19.265 | 18.173 | 10.106 | 1.00 | 33.09 | N |
| ATOM | 400 | CA  | ASP | A | 66 | 19.392 | 16.767 | 9.724  | 1.00 | 33.53 | C |
| ATOM | 401 | C   | ASP | A | 66 | 20.629 | 16.019 | 10.189 | 1.00 | 33.55 | C |
| ATOM | 402 | O   | ASP | A | 66 | 21.136 | 15.179 | 9.458  | 1.00 | 33.68 | O |
| ATOM | 403 | CB  | ASP | A | 66 | 19.339 | 16.653 | 8.192  | 1.00 | 33.55 | C |
| ATOM | 404 | CG  | ASP | A | 66 | 20.397 | 17.484 | 7.508  | 1.00 | 34.00 | C |
| ATOM | 405 | OD1 | ASP | A | 66 | 21.124 | 18.232 | 8.188  | 1.00 | 35.03 | O |
| ATOM | 406 | OD2 | ASP | A | 66 | 20.583 | 17.456 | 6.284  | 1.00 | 35.31 | O |
| ATOM | 407 | N   | THR | A | 67 | 21.107 | 16.264 | 11.397 | 1.00 | 33.83 | N |
| ATOM | 408 | CA  | THR | A | 67 | 22.286 | 15.540 | 11.845 | 1.00 | 33.70 | C |
| ATOM | 409 | C   | THR | A | 67 | 21.937 | 14.177 | 12.340 | 1.00 | 33.84 | C |
| ATOM | 410 | O   | THR | A | 67 | 22.808 | 13.340 | 12.431 | 1.00 | 34.42 | O |
| ATOM | 411 | CB  | THR | A | 67 | 22.951 | 16.215 | 13.020 | 1.00 | 33.66 | C |
| ATOM | 412 | OG1 | THR | A | 67 | 21.981 | 16.451 | 14.046 | 1.00 | 33.90 | O |
| ATOM | 413 | CG2 | THR | A | 67 | 23.472 | 17.562 | 12.674 | 1.00 | 33.56 | C |
| ATOM | 414 | N   | ASN | A | 68 | 20.686 | 13.954 | 12.719 | 1.00 | 34.00 | N |
| ATOM | 415 | CA  | ASN | A | 68 | 20.320 | 12.676 | 13.312 | 1.00 | 34.15 | C |
| ATOM | 416 | C   | ASN | A | 68 | 21.108 | 12.454 | 14.575 | 1.00 | 33.97 | C |
| ATOM | 417 | O   | ASN | A | 68 | 21.281 | 11.330 | 15.008 | 1.00 | 33.83 | O |
| ATOM | 418 | CB  | ASN | A | 68 | 20.653 | 11.531 | 12.375 | 1.00 | 34.26 | C |
| ATOM | 419 | CG  | ASN | A | 68 | 19.685 | 11.411 | 11.239 | 1.00 | 35.12 | C |
| ATOM | 420 | OD1 | ASN | A | 68 | 18.512 | 11.104 | 11.434 | 1.00 | 35.89 | O |
| ATOM | 421 | ND2 | ASN | A | 68 | 20.168 | 11.649 | 10.033 | 1.00 | 36.88 | N |
| ATOM | 422 | N   | LEU | A | 69 | 21.598 | 13.531 | 15.162 | 1.00 | 34.12 | N |
| ATOM | 423 | CA  | LEU | A | 69 | 22.446 | 13.419 | 16.334 | 1.00 | 34.19 | C |
| ATOM | 424 | C   | LEU | A | 69 | 21.836 | 12.562 | 17.440 | 1.00 | 34.16 | C |
| ATOM | 425 | O   | LEU | A | 69 | 22.538 | 11.737 | 18.039 | 1.00 | 33.75 | O |
| ATOM | 426 | CB  | LEU | A | 69 | 22.774 | 14.808 | 16.881 | 1.00 | 34.13 | C |
| ATOM | 427 | CG  | LEU | A | 69 | 23.652 | 14.795 | 18.125 | 1.00 | 34.10 | C |
| ATOM | 428 | CD1 | LEU | A | 69 | 24.978 | 14.105 | 17.854 | 1.00 | 34.66 | C |
| ATOM | 429 | CD2 | LEU | A | 69 | 23.883 | 16.183 | 18.582 | 1.00 | 33.94 | C |
| ATOM | 430 | N   | VAL | A | 70 | 20.555 | 12.783 | 17.732 | 1.00 | 34.15 | N |
| ATOM | 431 | CA  | VAL | A | 70 | 19.877 | 12.023 | 18.777 | 1.00 | 34.48 | C |
| ATOM | 432 | C   | VAL | A | 70 | 18.654 | 11.307 | 18.228 | 1.00 | 34.64 | C |
| ATOM | 433 | O   | VAL | A | 70 | 17.600 | 11.223 | 18.865 | 1.00 | 34.46 | O |
| ATOM | 434 | CB  | VAL | A | 70 | 19.540 | 12.899 | 20.003 | 1.00 | 34.61 | C |
| ATOM | 435 | CG1 | VAL | A | 70 | 20.808 | 13.555 | 20.519 | 1.00 | 35.04 | C |
| ATOM | 436 | CG2 | VAL | A | 70 | 18.493 | 13.939 | 19.706 | 1.00 | 34.21 | C |
| ATOM | 437 | N   | TYR | A | 71 | 18.833 | 10.762 | 17.033 | 1.00 | 34.98 | N |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 438 | CA  | TYR | A | 71 | 17.779 | 10.041 | 16.352 | 1.00 | 35.19 | C |
| ATOM | 439 | C   | TYR | A | 71 | 17.051 | 9.086  | 17.305 | 1.00 | 35.24 | C |
| ATOM | 440 | O   | TYR | A | 71 | 15.837 | 9.148  | 17.421 | 1.00 | 35.61 | O |
| ATOM | 441 | CB  | TYR | A | 71 | 18.337 | 9.291  | 15.137 | 1.00 | 35.26 | C |
| ATOM | 442 | CG  | TYR | A | 71 | 17.352 | 8.278  | 14.618 | 1.00 | 35.95 | C |
| ATOM | 443 | CD1 | TYR | A | 71 | 16.155 | 8.696  | 14.055 | 1.00 | 35.96 | C |
| ATOM | 444 | CD2 | TYR | A | 71 | 17.584 | 6.915  | 14.731 | 1.00 | 34.66 | C |
| ATOM | 445 | CE1 | TYR | A | 71 | 15.239 | 7.805  | 13.610 | 1.00 | 35.86 | C |
| ATOM | 446 | CE2 | TYR | A | 71 | 16.664 | 6.011  | 14.281 | 1.00 | 34.47 | C |
| ATOM | 447 | CZ  | TYR | A | 71 | 15.485 | 6.463  | 13.724 | 1.00 | 36.06 | C |
| ATOM | 448 | OH  | TYR | A | 71 | 14.518 | 5.589  | 13.248 | 1.00 | 38.92 | O |
| ATOM | 449 | N   | PRO | A | 72 | 17.774 | 8.211  | 17.993 | 1.00 | 35.15 | N |
| ATOM | 450 | CA  | PRO | A | 72 | 17.141 | 7.271  | 18.924 | 1.00 | 35.16 | C |
| ATOM | 451 | C   | PRO | A | 72 | 16.357 | 7.923  | 20.068 | 1.00 | 35.14 | C |
| ATOM | 452 | O   | PRO | A | 72 | 15.473 | 7.294  | 20.643 | 1.00 | 34.97 | O |
| ATOM | 453 | CB  | PRO | A | 72 | 18.327 | 6.475  | 19.487 | 1.00 | 35.18 | C |
| ATOM | 454 | CG  | PRO | A | 72 | 19.433 | 6.677  | 18.524 | 1.00 | 35.26 | C |
| ATOM | 455 | CD  | PRO | A | 72 | 19.233 | 8.031  | 17.938 | 1.00 | 35.29 | C |
| ATOM | 456 | N   | ALA | A | 73 | 16.657 | 9.169  | 20.401 | 1.00 | 35.18 | N |
| ATOM | 457 | CA  | ALA | A | 73 | 15.967 | 9.803  | 21.512 | 1.00 | 35.21 | C |
| ATOM | 458 | C   | ALA | A | 73 | 14.657 | 10.414 | 21.097 | 1.00 | 35.08 | C |
| ATOM | 459 | O   | ALA | A | 73 | 13.890 | 10.862 | 21.934 | 1.00 | 34.86 | O |
| ATOM | 460 | CB  | ALA | A | 73 | 16.829 | 10.864 | 22.135 | 1.00 | 35.37 | C |
| ATOM | 461 | N   | LEU | A | 74 | 14.370 | 10.434 | 19.812 | 1.00 | 35.25 | N |
| ATOM | 462 | CA  | LEU | A | 74 | 13.142 | 11.090 | 19.399 | 1.00 | 35.54 | C |
| ATOM | 463 | C   | LEU | A | 74 | 11.903 | 10.434 | 19.958 | 1.00 | 35.66 | C |
| ATOM | 464 | O   | LEU | A | 74 | 10.893 | 11.088 | 20.118 | 1.00 | 35.64 | O |
| ATOM | 465 | CB  | LEU | A | 74 | 13.044 | 11.190 | 17.894 | 1.00 | 35.31 | C |
| ATOM | 466 | CG  | LEU | A | 74 | 14.161 | 12.046 | 17.333 | 1.00 | 36.48 | C |
| ATOM | 467 | CD1 | LEU | A | 74 | 13.887 | 12.277 | 15.890 | 1.00 | 37.76 | C |
| ATOM | 468 | CD2 | LEU | A | 74 | 14.300 | 13.394 | 18.076 | 1.00 | 37.06 | C |
| ATOM | 469 | N   | LYS | A | 75 | 11.979 | 9.151  | 20.282 | 1.00 | 36.19 | N |
| ATOM | 470 | CA  | LYS | A | 75 | 10.795 | 8.453  | 20.767 | 1.00 | 36.36 | C |
| ATOM | 471 | C   | LYS | A | 75 | 10.566 | 8.710  | 22.246 | 1.00 | 36.85 | C |
| ATOM | 472 | O   | LYS | A | 75 | 9.491  | 8.437  | 22.765 | 1.00 | 37.12 | O |
| ATOM | 473 | CB  | LYS | A | 75 | 10.904 | 6.956  | 20.505 | 1.00 | 36.04 | C |
| ATOM | 474 | CG  | LYS | A | 75 | 12.060 | 6.284  | 21.216 | 1.00 | 35.77 | C |
| ATOM | 475 | CD  | LYS | A | 75 | 12.245 | 4.829  | 20.782 | 1.00 | 34.46 | C |
| ATOM | 476 | CE  | LYS | A | 75 | 13.720 | 4.460  | 20.710 | 1.00 | 33.42 | C |
| ATOM | 477 | NZ  | LYS | A | 75 | 14.375 | 4.536  | 22.036 | 1.00 | 32.34 | N |
| ATOM | 478 | N   | TRP | A | 76 | 11.578 | 9.244  | 22.920 | 1.00 | 37.24 | N |
| ATOM | 479 | CA  | TRP | A | 76 | 11.481 | 9.510  | 24.345 | 1.00 | 37.30 | C |
| ATOM | 480 | C   | TRP | A | 76 | 10.274 | 10.369 | 24.700 | 1.00 | 37.42 | C |
| ATOM | 481 | O   | TRP | A | 76 | 9.917  | 11.306 | 23.984 | 1.00 | 37.54 | O |
| ATOM | 482 | CB  | TRP | A | 76 | 12.728 | 10.247 | 24.838 | 1.00 | 37.12 | C |
| ATOM | 483 | CG  | TRP | A | 76 | 13.980 | 9.446  | 24.816 | 1.00 | 36.77 | C |
| ATOM | 484 | CD1 | TRP | A | 76 | 14.142 | 8.176  | 24.359 | 1.00 | 37.03 | C |
| ATOM | 485 | CD2 | TRP | A | 76 | 15.255 | 9.864  | 25.291 | 1.00 | 36.31 | C |
| ATOM | 486 | NE1 | TRP | A | 76 | 15.445 | 7.776  | 24.527 | 1.00 | 36.52 | N |
| ATOM | 487 | CE2 | TRP | A | 76 | 16.147 | 8.801  | 25.097 | 1.00 | 36.08 | C |
| ATOM | 488 | CE3 | TRP | A | 76 | 15.737 | 11.040 | 25.864 | 1.00 | 36.23 | C |
| ATOM | 489 | CZ2 | TRP | A | 76 | 17.480 | 8.881  | 25.443 | 1.00 | 36.27 | C |
| ATOM | 490 | CZ3 | TRP | A | 76 | 17.055 | 11.113 | 26.209 | 1.00 | 36.35 | C |
| ATOM | 491 | CH2 | TRP | A | 76 | 17.915 | 10.045 | 25.996 | 1.00 | 36.41 | C |
| ATOM | 492 | N   | ASP | A | 77 | 9.662  | 10.015 | 25.820 | 1.00 | 37.42 | N |
| ATOM | 493 | CA  | ASP | A | 77 | 8.591  | 10.768 | 26.435 | 1.00 | 37.36 | C |
| ATOM | 494 | C   | ASP | A | 77 | 8.707  | 10.370 | 27.907 | 1.00 | 37.09 | C |
| ATOM | 495 | O   | ASP | A | 77 | 9.628  | 9.647  | 28.260 | 1.00 | 37.04 | O |
| ATOM | 496 | CB  | ASP | A | 77 | 7.245  | 10.377 | 25.834 | 1.00 | 37.48 | C |
| ATOM | 497 | CG  | ASP | A | 77 | 6.990  | 8.888  | 25.903 | 1.00 | 38.01 | C |
| ATOM | 498 | OD1 | ASP | A | 77 | 7.704  | 8.191  | 26.658 | 1.00 | 38.42 | O |

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 499 | OD2 | ASP | A | 77 | 6.093  | 8.319  | 25.244 | 1.00 | 39.67 | O |
| ATOM | 500 | N   | LEU | A | 78 | 7.789  | 10.798 | 28.763 | 1.00 | 36.79 | N |
| ATOM | 501 | CA  | LEU | A | 78 | 7.913  | 10.496 | 30.182 | 1.00 | 36.49 | C |
| ATOM | 502 | C   | LEU | A | 78 | 7.729  | 9.026  | 30.464 | 1.00 | 36.62 | C |
| ATOM | 503 | O   | LEU | A | 78 | 8.456  | 8.426  | 31.260 | 1.00 | 36.50 | O |
| ATOM | 504 | CB  | LEU | A | 78 | 6.903  | 11.296 | 30.974 | 1.00 | 36.33 | C |
| ATOM | 505 | CG  | LEU | A | 78 | 7.119  | 12.796 | 30.863 | 1.00 | 36.49 | C |
| ATOM | 506 | CD1 | LEU | A | 78 | 6.008  | 13.510 | 31.594 | 1.00 | 36.63 | C |
| ATOM | 507 | CD2 | LEU | A | 78 | 8.494  | 13.194 | 31.399 | 1.00 | 36.10 | C |
| ATOM | 508 | N   | GLU | A | 79 | 6.748  | 8.433  | 29.815 | 1.00 | 36.81 | N |
| ATOM | 509 | CA  | GLU | A | 79 | 6.505  | 7.030  | 30.041 | 1.00 | 36.97 | C |
| ATOM | 510 | C   | GLU | A | 79 | 7.737  | 6.176  | 29.738 | 1.00 | 36.75 | C |
| ATOM | 511 | O   | GLU | A | 79 | 8.151  | 5.373  | 30.572 | 1.00 | 36.84 | O |
| ATOM | 512 | CB  | GLU | A | 79 | 5.323  | 6.560  | 29.214 | 1.00 | 37.25 | C |
| ATOM | 513 | CG  | GLU | A | 79 | 4.937  | 5.137  | 29.540 | 1.00 | 37.93 | C |
| ATOM | 514 | CD  | GLU | A | 79 | 3.729  | 4.681  | 28.768 | 1.00 | 38.61 | C |
| ATOM | 515 | OE1 | GLU | A | 79 | 3.381  | 5.352  | 27.775 | 1.00 | 38.32 | O |
| ATOM | 516 | OE2 | GLU | A | 79 | 3.131  | 3.654  | 29.166 | 1.00 | 40.10 | O |
| ATOM | 517 | N   | TYR | A | 80 | 8.318  | 6.337  | 28.553 | 1.00 | 36.50 | N |
| ATOM | 518 | CA  | TYR | A | 80 | 9.489  | 5.549  | 28.176 | 1.00 | 36.32 | C |
| ATOM | 519 | C   | TYR | A | 80 | 10.644 | 5.804  | 29.123 | 1.00 | 36.27 | C |
| ATOM | 520 | O   | TYR | A | 80 | 11.343 | 4.872  | 29.516 | 1.00 | 36.15 | O |
| ATOM | 521 | CB  | TYR | A | 80 | 9.921  | 5.889  | 26.751 | 1.00 | 36.39 | C |
| ATOM | 522 | CG  | TYR | A | 80 | 11.180 | 5.202  | 26.228 | 1.00 | 36.06 | C |
| ATOM | 523 | CD1 | TYR | A | 80 | 11.100 | 4.000  | 25.557 | 1.00 | 36.22 | C |
| ATOM | 524 | CD2 | TYR | A | 80 | 12.432 | 5.793  | 26.349 | 1.00 | 35.91 | C |
| ATOM | 525 | CE1 | TYR | A | 80 | 12.225 | 3.380  | 25.051 | 1.00 | 36.52 | C |
| ATOM | 526 | CE2 | TYR | A | 80 | 13.568 | 5.179  | 25.844 | 1.00 | 36.04 | C |
| ATOM | 527 | CZ  | TYR | A | 80 | 13.454 | 3.967  | 25.190 | 1.00 | 36.46 | C |
| ATOM | 528 | OH  | TYR | A | 80 | 14.561 | 3.321  | 24.673 | 1.00 | 35.81 | O |
| ATOM | 529 | N   | LEU | A | 81 | 10.846 | 7.064  | 29.493 | 1.00 | 36.13 | N |
| ATOM | 530 | CA  | LEU | A | 81 | 11.971 | 7.408  | 30.353 | 1.00 | 36.22 | C |
| ATOM | 531 | C   | LEU | A | 81 | 11.777 | 6.827  | 31.747 | 1.00 | 36.13 | C |
| ATOM | 532 | O   | LEU | A | 81 | 12.706 | 6.259  | 32.325 | 1.00 | 35.90 | O |
| ATOM | 533 | CB  | LEU | A | 81 | 12.208 | 8.930  | 30.406 | 1.00 | 36.22 | C |
| ATOM | 534 | CG  | LEU | A | 81 | 12.774 | 9.568  | 29.121 | 1.00 | 36.35 | C |
| ATOM | 535 | CD1 | LEU | A | 81 | 12.880 | 11.055 | 29.274 | 1.00 | 36.49 | C |
| ATOM | 536 | CD2 | LEU | A | 81 | 14.132 | 9.017  | 28.718 | 1.00 | 36.18 | C |
| ATOM | 537 | N   | GLN | A | 82 | 10.569 | 6.956  | 32.280 | 1.00 | 36.15 | N |
| ATOM | 538 | CA  | GLN | A | 82 | 10.284 | 6.424  | 33.597 | 1.00 | 36.29 | C |
| ATOM | 539 | C   | GLN | A | 82 | 10.575 | 4.927  | 33.605 | 1.00 | 36.25 | C |
| ATOM | 540 | O   | GLN | A | 82 | 11.210 | 4.408  | 34.515 | 1.00 | 35.96 | O |
| ATOM | 541 | CB  | GLN | A | 82 | 8.838  | 6.710  | 33.976 | 1.00 | 36.38 | C |
| ATOM | 542 | CG  | GLN | A | 82 | 8.418  | 6.080  | 35.279 | 1.00 | 37.00 | C |
| ATOM | 543 | CD  | GLN | A | 82 | 7.191  | 6.740  | 35.872 | 1.00 | 37.85 | C |
| ATOM | 544 | OE1 | GLN | A | 82 | 6.640  | 7.676  | 35.295 | 1.00 | 38.24 | O |
| ATOM | 545 | NE2 | GLN | A | 82 | 6.754  | 6.247  | 37.020 | 1.00 | 38.93 | N |
| ATOM | 546 | N   | GLU | A | 83 | 10.136 | 4.240  | 32.560 | 1.00 | 36.46 | N |
| ATOM | 547 | CA  | GLU | A | 83 | 10.366 | 2.807  | 32.451 | 1.00 | 36.59 | C |
| ATOM | 548 | C   | GLU | A | 83 | 11.843 | 2.424  | 32.307 | 1.00 | 36.50 | C |
| ATOM | 549 | O   | GLU | A | 83 | 12.228 | 1.321  | 32.677 | 1.00 | 36.55 | O |
| ATOM | 550 | CB  | GLU | A | 83 | 9.568  | 2.237  | 31.271 | 1.00 | 36.57 | C |
| ATOM | 551 | CG  | GLU | A | 83 | 9.497  | 0.714  | 31.239 | 1.00 | 36.95 | C |
| ATOM | 552 | CD  | GLU | A | 83 | 8.732  | 0.107  | 32.416 | 1.00 | 37.61 | C |
| ATOM | 553 | OE1 | GLU | A | 83 | 7.922  | 0.815  | 33.050 | 1.00 | 37.88 | O |
| ATOM | 554 | OE2 | GLU | A | 83 | 8.938  | -1.090 | 32.719 | 1.00 | 37.54 | O |
| ATOM | 555 | N   | ASN | A | 84 | 12.680 | 3.324  | 31.805 | 1.00 | 36.58 | N |
| ATOM | 556 | CA  | ASN | A | 84 | 14.049 | 2.936  | 31.476 | 1.00 | 36.62 | C |
| ATOM | 557 | C   | ASN | A | 84 | 15.210 | 3.749  | 32.001 | 1.00 | 36.66 | C |
| ATOM | 558 | O   | ASN | A | 84 | 16.349 | 3.310  | 31.900 | 1.00 | 36.62 | O |
| ATOM | 559 | CB  | ASN | A | 84 | 14.211 | 2.936  | 29.960 | 1.00 | 36.62 | C |



|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 560 | CG  | ASN | A | 84 | 13.362 | 1.902  | 29.286 | 1.00 | 36.37 | C |
| ATOM | 561 | OD1 | ASN | A | 84 | 13.352 | 0.733  | 29.683 | 1.00 | 36.46 | O |
| ATOM | 562 | ND2 | ASN | A | 84 | 12.644 | 2.317  | 28.247 | 1.00 | 35.65 | N |
| ATOM | 563 | N   | ILE | A | 85 | 14.975 | 4.920  | 32.557 | 1.00 | 36.80 | N |
| ATOM | 564 | CA  | ILE | A | 85 | 16.125 | 5.730  | 32.885 | 1.00 | 37.13 | C |
| ATOM | 565 | C   | ILE | A | 85 | 16.834 | 5.365  | 34.180 | 1.00 | 37.28 | C |
| ATOM | 566 | O   | ILE | A | 85 | 17.793 | 6.022  | 34.568 | 1.00 | 37.74 | O |
| ATOM | 567 | CB  | ILE | A | 85 | 15.752 | 7.184  | 32.874 | 1.00 | 37.21 | C |
| ATOM | 568 | CG1 | ILE | A | 85 | 16.958 | 8.009  | 32.445 | 1.00 | 37.55 | C |
| ATOM | 569 | CG2 | ILE | A | 85 | 15.241 | 7.593  | 34.222 | 1.00 | 37.38 | C |
| ATOM | 570 | CD1 | ILE | A | 85 | 16.623 | 9.467  | 32.195 | 1.00 | 37.68 | C |
| ATOM | 571 | N   | GLY | A | 86 | 16.383 | 4.326  | 34.855 | 1.00 | 37.29 | N |
| ATOM | 572 | CA  | GLY | A | 86 | 17.089 | 3.892  | 36.038 | 1.00 | 37.39 | C |
| ATOM | 573 | C   | GLY | A | 86 | 16.553 | 4.496  | 37.308 | 1.00 | 37.43 | C |
| ATOM | 574 | O   | GLY | A | 86 | 15.583 | 5.265  | 37.290 | 1.00 | 37.34 | O |
| ATOM | 575 | N   | ASN | A | 87 | 17.212 | 4.167  | 38.414 | 1.00 | 37.34 | N |
| ATOM | 576 | CA  | ASN | A | 87 | 16.750 | 4.602  | 39.716 | 1.00 | 37.42 | C |
| ATOM | 577 | C   | ASN | A | 87 | 17.701 | 5.603  | 40.357 | 1.00 | 37.39 | C |
| ATOM | 578 | O   | ASN | A | 87 | 17.740 | 5.742  | 41.578 | 1.00 | 37.39 | O |
| ATOM | 579 | CB  | ASN | A | 87 | 16.545 | 3.399  | 40.612 | 1.00 | 37.40 | C |
| ATOM | 580 | N   | GLY | A | 88 | 18.451 | 6.321  | 39.529 | 1.00 | 37.47 | N |
| ATOM | 581 | CA  | GLY | A | 88 | 19.405 | 7.296  | 40.028 | 1.00 | 37.41 | C |
| ATOM | 582 | C   | GLY | A | 88 | 18.686 | 8.554  | 40.450 | 1.00 | 37.30 | C |
| ATOM | 583 | O   | GLY | A | 88 | 17.500 | 8.709  | 40.171 | 1.00 | 37.36 | O |
| ATOM | 584 | N   | ASP | A | 89 | 19.390 | 9.453  | 41.125 | 1.00 | 37.26 | N |
| ATOM | 585 | CA  | ASP | A | 89 | 18.780 | 10.716 | 41.531 | 1.00 | 37.21 | C |
| ATOM | 586 | C   | ASP | A | 89 | 18.726 | 11.681 | 40.355 | 1.00 | 36.91 | C |
| ATOM | 587 | O   | ASP | A | 89 | 19.607 | 11.654 | 39.500 | 1.00 | 36.62 | O |
| ATOM | 588 | CB  | ASP | A | 89 | 19.563 | 11.346 | 42.680 | 1.00 | 37.24 | C |
| ATOM | 589 | CG  | ASP | A | 89 | 19.277 | 10.690 | 44.000 | 1.00 | 37.24 | C |
| ATOM | 590 | OD1 | ASP | A | 89 | 18.398 | 9.802  | 44.044 | 1.00 | 37.14 | O |
| ATOM | 591 | OD2 | ASP | A | 89 | 19.876 | 11.002 | 45.047 | 1.00 | 37.98 | O |
| ATOM | 592 | N   | PHE | A | 90 | 17.667 | 12.492 | 40.295 | 1.00 | 36.88 | N |
| ATOM | 593 | CA  | PHE | A | 90 | 17.554 | 13.570 | 39.298 | 1.00 | 36.87 | C |
| ATOM | 594 | C   | PHE | A | 90 | 17.327 | 14.926 | 39.942 | 1.00 | 36.79 | C |
| ATOM | 595 | O   | PHE | A | 90 | 16.455 | 15.080 | 40.795 | 1.00 | 36.69 | O |
| ATOM | 596 | CB  | PHE | A | 90 | 16.420 | 13.308 | 38.321 | 1.00 | 36.70 | C |
| ATOM | 597 | CG  | PHE | A | 90 | 16.712 | 12.210 | 37.371 | 1.00 | 36.83 | C |
| ATOM | 598 | CD1 | PHE | A | 90 | 16.551 | 10.901 | 37.757 | 1.00 | 36.07 | C |
| ATOM | 599 | CD2 | PHE | A | 90 | 17.191 | 12.479 | 36.102 | 1.00 | 37.27 | C |
| ATOM | 600 | CE1 | PHE | A | 90 | 16.827 | 9.885  | 36.899 | 1.00 | 35.81 | C |
| ATOM | 601 | CE2 | PHE | A | 90 | 17.475 | 11.449 | 35.238 | 1.00 | 36.82 | C |
| ATOM | 602 | CZ  | PHE | A | 90 | 17.291 | 10.150 | 35.642 | 1.00 | 36.06 | C |
| ATOM | 603 | N   | SER | A | 91 | 18.123 | 15.905 | 39.529 | 1.00 | 36.92 | N |
| ATOM | 604 | CA  | SER | A | 91 | 17.971 | 17.266 | 40.027 | 1.00 | 36.99 | C |
| ATOM | 605 | C   | SER | A | 91 | 16.738 | 17.923 | 39.428 | 1.00 | 37.10 | C |
| ATOM | 606 | O   | SER | A | 91 | 16.586 | 17.985 | 38.206 | 1.00 | 36.78 | O |
| ATOM | 607 | CB  | SER | A | 91 | 19.200 | 18.105 | 39.699 | 1.00 | 36.86 | C |
| ATOM | 608 | OG  | SER | A | 91 | 20.350 | 17.616 | 40.358 | 1.00 | 36.54 | O |
| ATOM | 609 | N   | VAL | A | 92 | 15.857 | 18.402 | 40.303 | 1.00 | 37.42 | N |
| ATOM | 610 | CA  | VAL | A | 92 | 14.660 | 19.106 | 39.876 | 1.00 | 37.75 | C |
| ATOM | 611 | C   | VAL | A | 92 | 14.509 | 20.468 | 40.545 | 1.00 | 38.10 | C |
| ATOM | 612 | O   | VAL | A | 92 | 14.472 | 20.589 | 41.768 | 1.00 | 38.08 | O |
| ATOM | 613 | CB  | VAL | A | 92 | 13.406 | 18.303 | 40.159 | 1.00 | 37.63 | C |
| ATOM | 614 | CG1 | VAL | A | 92 | 12.197 | 19.034 | 39.621 | 1.00 | 37.42 | C |
| ATOM | 615 | CG2 | VAL | A | 92 | 13.515 | 16.946 | 39.527 | 1.00 | 37.78 | C |
| ATOM | 616 | N   | TYR | A | 93 | 14.384 | 21.487 | 39.709 | 1.00 | 38.59 | N |
| ATOM | 617 | CA  | TYR | A | 93 | 14.220 | 22.849 | 40.166 | 1.00 | 38.91 | C |
| ATOM | 618 | C   | TYR | A | 93 | 12.784 | 23.173 | 40.219 | 1.00 | 39.41 | C |
| ATOM | 619 | O   | TYR | A | 93 | 12.019 | 22.786 | 39.343 | 1.00 | 39.64 | O |
| ATOM | 620 | CB  | TYR | A | 93 | 14.883 | 23.799 | 39.202 | 1.00 | 38.84 | C |



|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 621 | CG  | TYR | A | 93  | 16.332 | 23.588 | 39.288 | 1.00 | 38.25 | C |
| ATOM | 622 | CD1 | TYR | A | 93  | 17.044 | 24.122 | 40.334 | 1.00 | 38.21 | C |
| ATOM | 623 | CD2 | TYR | A | 93  | 16.968 | 22.750 | 38.415 | 1.00 | 37.50 | C |
| ATOM | 624 | CE1 | TYR | A | 93  | 18.362 | 23.893 | 40.464 | 1.00 | 37.90 | C |
| ATOM | 625 | CE2 | TYR | A | 93  | 18.287 | 22.512 | 38.534 | 1.00 | 37.82 | C |
| ATOM | 626 | CZ  | TYR | A | 93  | 18.987 | 23.090 | 39.557 | 1.00 | 37.78 | C |
| ATOM | 627 | OH  | TYR | A | 93  | 20.322 | 22.836 | 39.677 | 1.00 | 39.39 | O |
| ATOM | 628 | N   | SER | A | 94  | 12.422 | 23.935 | 41.228 | 1.00 | 40.00 | N |
| ATOM | 629 | CA  | SER | A | 94  | 11.043 | 24.274 | 41.416 | 1.00 | 40.51 | C |
| ATOM | 630 | C   | SER | A | 94  | 11.020 | 25.773 | 41.426 | 1.00 | 40.68 | C |
| ATOM | 631 | O   | SER | A | 94  | 11.962 | 26.384 | 41.896 | 1.00 | 41.00 | O |
| ATOM | 632 | CB  | SER | A | 94  | 10.539 | 23.693 | 42.730 | 1.00 | 40.58 | C |
| ATOM | 633 | OG  | SER | A | 94  | 9.139  | 23.874 | 42.858 | 1.00 | 41.30 | O |
| ATOM | 634 | N   | ALA | A | 95  | 9.974  | 26.374 | 40.878 | 1.00 | 40.87 | N |
| ATOM | 635 | CA  | ALA | A | 95  | 9.899  | 27.824 | 40.856 | 1.00 | 40.91 | C |
| ATOM | 636 | C   | ALA | A | 95  | 8.483  | 28.343 | 40.826 | 1.00 | 41.03 | C |
| ATOM | 637 | O   | ALA | A | 95  | 7.573  | 27.699 | 40.309 | 1.00 | 41.09 | O |
| ATOM | 638 | CB  | ALA | A | 95  | 10.630 | 28.350 | 39.668 | 1.00 | 40.93 | C |
| ATOM | 639 | N   | SER | A | 96  | 8.328  | 29.549 | 41.350 | 1.00 | 41.12 | N |
| ATOM | 640 | CA  | SER | A | 96  | 7.034  | 30.200 | 41.413 | 1.00 | 41.05 | C |
| ATOM | 641 | C   | SER | A | 96  | 6.834  | 31.208 | 40.305 | 1.00 | 40.72 | C |
| ATOM | 642 | O   | SER | A | 96  | 5.833  | 31.912 | 40.277 | 1.00 | 40.86 | O |
| ATOM | 643 | CB  | SER | A | 96  | 6.902  | 30.938 | 42.731 | 1.00 | 41.16 | C |
| ATOM | 644 | OG  | SER | A | 96  | 5.767  | 31.779 | 42.693 | 1.00 | 41.90 | O |
| ATOM | 645 | N   | THR | A | 97  | 7.808  | 31.314 | 39.423 | 1.00 | 40.34 | N |
| ATOM | 646 | CA  | THR | A | 97  | 7.710  | 32.209 | 38.292 | 1.00 | 40.18 | C |
| ATOM | 647 | C   | THR | A | 97  | 8.073  | 31.368 | 37.113 | 1.00 | 39.72 | C |
| ATOM | 648 | O   | THR | A | 97  | 8.582  | 30.274 | 37.279 | 1.00 | 39.83 | O |
| ATOM | 649 | CB  | THR | A | 97  | 8.732  | 33.336 | 38.393 | 1.00 | 40.49 | C |
| ATOM | 650 | OG1 | THR | A | 97  | 8.905  | 33.946 | 37.105 | 1.00 | 41.00 | O |
| ATOM | 651 | CG2 | THR | A | 97  | 10.145 | 32.779 | 38.718 | 1.00 | 40.86 | C |
| ATOM | 652 | N   | HIS | A | 98  | 7.862  | 31.874 | 35.915 | 1.00 | 39.32 | N |
| ATOM | 653 | CA  | HIS | A | 98  | 8.257  | 31.112 | 34.754 | 1.00 | 39.12 | C |
| ATOM | 654 | C   | HIS | A | 98  | 9.765  | 31.163 | 34.543 | 1.00 | 39.41 | C |
| ATOM | 655 | O   | HIS | A | 98  | 10.299 | 30.423 | 33.711 | 1.00 | 39.15 | O |
| ATOM | 656 | CB  | HIS | A | 98  | 7.576  | 31.646 | 33.516 | 1.00 | 38.95 | C |
| ATOM | 657 | CG  | HIS | A | 98  | 7.807  | 33.104 | 33.290 | 1.00 | 38.64 | C |
| ATOM | 658 | ND1 | HIS | A | 98  | 7.095  | 34.081 | 33.950 | 1.00 | 37.36 | N |
| ATOM | 659 | CD2 | HIS | A | 98  | 8.672  | 33.753 | 32.477 | 1.00 | 38.57 | C |
| ATOM | 660 | CE1 | HIS | A | 98  | 7.509  | 35.268 | 33.550 | 1.00 | 37.33 | C |
| ATOM | 661 | NE2 | HIS | A | 98  | 8.463  | 35.098 | 32.654 | 1.00 | 37.37 | N |
| ATOM | 662 | N   | LYS | A | 99  | 10.452 | 32.021 | 35.294 | 1.00 | 39.52 | N |
| ATOM | 663 | CA  | LYS | A | 99  | 11.881 | 32.184 | 35.105 | 1.00 | 39.98 | C |
| ATOM | 664 | C   | LYS | A | 99  | 12.749 | 31.364 | 36.029 | 1.00 | 40.38 | C |
| ATOM | 665 | O   | LYS | A | 99  | 12.744 | 31.554 | 37.246 | 1.00 | 40.33 | O |
| ATOM | 666 | CB  | LYS | A | 99  | 12.281 | 33.631 | 35.297 | 1.00 | 40.10 | C |
| ATOM | 667 | CG  | LYS | A | 99  | 11.814 | 34.527 | 34.219 | 1.00 | 40.15 | C |
| ATOM | 668 | CD  | LYS | A | 99  | 12.537 | 35.820 | 34.337 | 1.00 | 40.36 | C |
| ATOM | 669 | CE  | LYS | A | 99  | 11.725 | 36.835 | 35.072 | 1.00 | 41.10 | C |
| ATOM | 670 | NZ  | LYS | A | 99  | 10.975 | 37.655 | 34.074 | 1.00 | 41.52 | N |
| ATOM | 671 | N   | PHE | A | 100 | 13.541 | 30.486 | 35.433 | 1.00 | 40.77 | N |
| ATOM | 672 | CA  | PHE | A | 100 | 14.450 | 29.665 | 36.201 | 1.00 | 41.12 | C |
| ATOM | 673 | C   | PHE | A | 100 | 15.893 | 30.159 | 36.218 | 1.00 | 41.78 | C |
| ATOM | 674 | O   | PHE | A | 100 | 16.808 | 29.463 | 35.765 | 1.00 | 42.13 | O |
| ATOM | 675 | CB  | PHE | A | 100 | 14.418 | 28.255 | 35.658 | 1.00 | 40.86 | C |
| ATOM | 676 | CG  | PHE | A | 100 | 13.211 | 27.494 | 36.060 | 1.00 | 40.53 | C |
| ATOM | 677 | CD1 | PHE | A | 100 | 12.040 | 27.604 | 35.344 | 1.00 | 39.76 | C |
| ATOM | 678 | CD2 | PHE | A | 100 | 13.249 | 26.666 | 37.159 | 1.00 | 39.54 | C |
| ATOM | 679 | CE1 | PHE | A | 100 | 10.942 | 26.890 | 35.707 | 1.00 | 39.56 | C |
| ATOM | 680 | CE2 | PHE | A | 100 | 12.155 | 25.955 | 37.526 | 1.00 | 39.79 | C |
| ATOM | 681 | CZ  | PHE | A | 100 | 10.995 | 26.064 | 36.802 | 1.00 | 39.91 | C |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 682 | N   | LEU | A | 101 | 16.124 | 31.347 | 36.747 | 1.00 | 42.23 | N |
| ATOM | 683 | CA  | LEU | A | 101 | 17.501 | 31.800 | 36.868 | 1.00 | 42.74 | C |
| ATOM | 684 | C   | LEU | A | 101 | 18.429 | 30.780 | 37.567 | 1.00 | 43.27 | C |
| ATOM | 685 | O   | LEU | A | 101 | 18.213 | 30.392 | 38.736 | 1.00 | 43.22 | O |
| ATOM | 686 | CB  | LEU | A | 101 | 17.549 | 33.097 | 37.657 | 1.00 | 42.90 | C |
| ATOM | 687 | CG  | LEU | A | 101 | 18.900 | 33.800 | 37.793 | 1.00 | 43.35 | C |
| ATOM | 688 | CD1 | LEU | A | 101 | 19.441 | 34.288 | 36.455 | 1.00 | 43.59 | C |
| ATOM | 689 | CD2 | LEU | A | 101 | 18.703 | 34.967 | 38.724 | 1.00 | 43.91 | C |
| ATOM | 690 | N   | TYR | A | 102 | 19.470 | 30.379 | 36.836 | 1.00 | 43.59 | N |
| ATOM | 691 | CA  | TYR | A | 102 | 20.547 | 29.522 | 37.340 | 1.00 | 43.71 | C |
| ATOM | 692 | C   | TYR | A | 102 | 21.380 | 30.186 | 38.460 | 1.00 | 43.57 | C |
| ATOM | 693 | O   | TYR | A | 102 | 21.746 | 31.364 | 38.343 | 1.00 | 44.09 | O |
| ATOM | 694 | CB  | TYR | A | 102 | 21.531 | 29.218 | 36.193 | 1.00 | 43.90 | C |
| ATOM | 695 | CG  | TYR | A | 102 | 22.703 | 28.421 | 36.700 | 1.00 | 44.68 | C |
| ATOM | 696 | CD1 | TYR | A | 102 | 22.553 | 27.080 | 37.033 | 1.00 | 44.29 | C |
| ATOM | 697 | CD2 | TYR | A | 102 | 23.935 | 29.023 | 36.918 | 1.00 | 44.88 | C |
| ATOM | 698 | CE1 | TYR | A | 102 | 23.602 | 26.358 | 37.541 | 1.00 | 44.98 | C |
| ATOM | 699 | CE2 | TYR | A | 102 | 24.987 | 28.309 | 37.422 | 1.00 | 45.44 | C |
| ATOM | 700 | CZ  | TYR | A | 102 | 24.826 | 26.984 | 37.735 | 1.00 | 45.86 | C |
| ATOM | 701 | OH  | TYR | A | 102 | 25.922 | 26.313 | 38.237 | 1.00 | 47.07 | O |
| ATOM | 702 | N   | TYR | A | 103 | 21.704 | 29.451 | 39.523 | 1.00 | 42.91 | N |
| ATOM | 703 | CA  | TYR | A | 103 | 22.642 | 29.970 | 40.527 | 1.00 | 42.67 | C |
| ATOM | 704 | C   | TYR | A | 103 | 23.561 | 28.895 | 41.102 | 1.00 | 41.98 | C |
| ATOM | 705 | O   | TYR | A | 103 | 23.165 | 27.768 | 41.351 | 1.00 | 41.99 | O |
| ATOM | 706 | CB  | TYR | A | 103 | 21.922 | 30.638 | 41.670 | 1.00 | 42.83 | C |
| ATOM | 707 | CG  | TYR | A | 103 | 20.974 | 29.692 | 42.265 | 1.00 | 44.33 | C |
| ATOM | 708 | CD1 | TYR | A | 103 | 19.770 | 29.454 | 41.646 | 1.00 | 46.69 | C |
| ATOM | 709 | CD2 | TYR | A | 103 | 21.306 | 28.959 | 43.390 | 1.00 | 45.99 | C |
| ATOM | 710 | CE1 | TYR | A | 103 | 18.880 | 28.539 | 42.147 | 1.00 | 47.83 | C |
| ATOM | 711 | CE2 | TYR | A | 103 | 20.426 | 28.045 | 43.917 | 1.00 | 47.23 | C |
| ATOM | 712 | CZ  | TYR | A | 103 | 19.203 | 27.836 | 43.284 | 1.00 | 48.65 | C |
| ATOM | 713 | OH  | TYR | A | 103 | 18.287 | 26.921 | 43.774 | 1.00 | 51.36 | O |
| ATOM | 714 | N   | ASP | A | 104 | 24.786 | 29.300 | 41.369 | 1.00 | 41.25 | N |
| ATOM | 715 | CA  | ASP | A | 104 | 25.829 | 28.399 | 41.764 | 1.00 | 40.65 | C |
| ATOM | 716 | C   | ASP | A | 104 | 25.924 | 28.335 | 43.267 | 1.00 | 40.45 | C |
| ATOM | 717 | O   | ASP | A | 104 | 26.430 | 29.240 | 43.924 | 1.00 | 40.13 | O |
| ATOM | 718 | CB  | ASP | A | 104 | 27.110 | 28.904 | 41.142 | 1.00 | 40.60 | C |
| ATOM | 719 | CG  | ASP | A | 104 | 28.306 | 28.117 | 41.548 | 1.00 | 41.02 | C |
| ATOM | 720 | OD1 | ASP | A | 104 | 28.270 | 27.482 | 42.629 | 1.00 | 42.21 | O |
| ATOM | 721 | OD2 | ASP | A | 104 | 29.337 | 28.095 | 40.838 | 1.00 | 40.68 | O |
| ATOM | 722 | N   | GLU | A | 105 | 25.446 | 27.222 | 43.801 | 1.00 | 40.41 | N |
| ATOM | 723 | CA  | GLU | A | 105 | 25.368 | 27.029 | 45.231 | 1.00 | 40.21 | C |
| ATOM | 724 | C   | GLU | A | 105 | 26.734 | 27.234 | 45.895 | 1.00 | 39.89 | C |
| ATOM | 725 | O   | GLU | A | 105 | 26.803 | 27.738 | 47.021 | 1.00 | 39.65 | O |
| ATOM | 726 | CB  | GLU | A | 105 | 24.769 | 25.643 | 45.528 | 1.00 | 40.44 | C |
| ATOM | 727 | CG  | GLU | A | 105 | 23.247 | 25.572 | 45.351 | 1.00 | 41.43 | C |
| ATOM | 728 | CD  | GLU | A | 105 | 22.708 | 24.150 | 45.207 | 1.00 | 42.48 | C |
| ATOM | 729 | OE1 | GLU | A | 105 | 23.138 | 23.269 | 45.986 | 1.00 | 43.10 | O |
| ATOM | 730 | OE2 | GLU | A | 105 | 21.842 | 23.914 | 44.322 | 1.00 | 42.00 | O |
| ATOM | 731 | N   | LYS | A | 106 | 27.824 | 26.899 | 45.204 | 1.00 | 39.58 | N |
| ATOM | 732 | CA  | LYS | A | 106 | 29.141 | 27.042 | 45.831 | 1.00 | 39.58 | C |
| ATOM | 733 | C   | LYS | A | 106 | 29.427 | 28.469 | 46.190 | 1.00 | 39.64 | C |
| ATOM | 734 | O   | LYS | A | 106 | 30.165 | 28.730 | 47.128 | 1.00 | 39.93 | O |
| ATOM | 735 | CB  | LYS | A | 106 | 30.302 | 26.592 | 44.945 | 1.00 | 39.49 | C |
| ATOM | 736 | CG  | LYS | A | 106 | 30.444 | 25.096 | 44.731 | 1.00 | 39.29 | C |
| ATOM | 737 | N   | LYS | A | 107 | 28.856 | 29.397 | 45.438 | 1.00 | 39.68 | N |
| ATOM | 738 | CA  | LYS | A | 107 | 29.140 | 30.794 | 45.663 | 1.00 | 39.58 | C |
| ATOM | 739 | C   | LYS | A | 107 | 28.151 | 31.452 | 46.607 | 1.00 | 40.18 | C |
| ATOM | 740 | O   | LYS | A | 107 | 28.279 | 32.637 | 46.883 | 1.00 | 40.30 | O |
| ATOM | 741 | CB  | LYS | A | 107 | 29.161 | 31.531 | 44.325 | 1.00 | 39.46 | C |
| ATOM | 742 | CG  | LYS | A | 107 | 30.390 | 31.199 | 43.455 | 1.00 | 38.46 | C |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 743 | CD  | LYS | A | 107 | 30.299 | 31.737 | 42.029 | 1.00 | 36.98 | C |
| ATOM | 744 | CE  | LYS | A | 107 | 31.643 | 31.632 | 41.292 | 1.00 | 36.36 | C |
| ATOM | 745 | NZ  | LYS | A | 107 | 31.553 | 31.935 | 39.819 | 1.00 | 35.12 | N |
| ATOM | 746 | N   | MET | A | 108 | 27.197 | 30.697 | 47.148 | 1.00 | 40.92 | N |
| ATOM | 747 | CA  | MET | A | 108 | 26.165 | 31.316 | 47.978 | 1.00 | 41.42 | C |
| ATOM | 748 | C   | MET | A | 108 | 26.675 | 31.937 | 49.258 | 1.00 | 42.03 | C |
| ATOM | 749 | O   | MET | A | 108 | 26.142 | 32.952 | 49.704 | 1.00 | 42.33 | O |
| ATOM | 750 | CB  | MET | A | 108 | 25.006 | 30.366 | 48.210 | 1.00 | 41.31 | C |
| ATOM | 751 | CG  | MET | A | 108 | 24.285 | 30.179 | 46.892 | 1.00 | 41.95 | C |
| ATOM | 752 | SD  | MET | A | 108 | 22.861 | 29.100 | 46.846 | 1.00 | 43.29 | S |
| ATOM | 753 | CE  | MET | A | 108 | 21.737 | 30.010 | 48.064 | 1.00 | 43.04 | C |
| ATOM | 754 | N   | ALA | A | 109 | 27.737 | 31.382 | 49.816 | 1.00 | 42.84 | N |
| ATOM | 755 | CA  | ALA | A | 109 | 28.282 | 31.912 | 51.064 | 1.00 | 43.65 | C |
| ATOM | 756 | C   | ALA | A | 109 | 28.655 | 33.387 | 50.963 | 1.00 | 44.40 | C |
| ATOM | 757 | O   | ALA | A | 109 | 28.321 | 34.195 | 51.823 | 1.00 | 44.44 | O |
| ATOM | 758 | CB  | ALA | A | 109 | 29.486 | 31.107 | 51.476 | 1.00 | 43.66 | C |
| ATOM | 759 | N   | ASN | A | 110 | 29.332 | 33.729 | 49.882 | 1.00 | 45.46 | N |
| ATOM | 760 | CA  | ASN | A | 110 | 29.817 | 35.084 | 49.665 | 1.00 | 46.25 | C |
| ATOM | 761 | C   | ASN | A | 110 | 28.789 | 36.154 | 49.317 | 1.00 | 46.26 | C |
| ATOM | 762 | O   | ASN | A | 110 | 29.163 | 37.304 | 49.066 | 1.00 | 46.51 | O |
| ATOM | 763 | CB  | ASN | A | 110 | 30.841 | 35.036 | 48.543 | 1.00 | 46.62 | C |
| ATOM | 764 | CG  | ASN | A | 110 | 32.024 | 34.145 | 48.886 | 1.00 | 47.94 | C |
| ATOM | 765 | OD1 | ASN | A | 110 | 32.474 | 34.093 | 50.045 | 1.00 | 48.12 | O |
| ATOM | 766 | ND2 | ASN | A | 110 | 32.530 | 33.432 | 47.883 | 1.00 | 48.75 | N |
| ATOM | 767 | N   | PHE | A | 111 | 27.517 | 35.786 | 49.228 | 1.00 | 46.12 | N |
| ATOM | 768 | CA  | PHE | A | 111 | 26.470 | 36.795 | 49.057 | 1.00 | 45.97 | C |
| ATOM | 769 | C   | PHE | A | 111 | 25.267 | 36.385 | 49.889 | 1.00 | 46.17 | C |
| ATOM | 770 | O   | PHE | A | 111 | 24.217 | 36.002 | 49.361 | 1.00 | 46.25 | O |
| ATOM | 771 | CB  | PHE | A | 111 | 26.072 | 36.978 | 47.599 | 1.00 | 45.55 | C |
| ATOM | 772 | CG  | PHE | A | 111 | 27.076 | 37.718 | 46.777 | 1.00 | 44.32 | C |
| ATOM | 773 | CD1 | PHE | A | 111 | 28.269 | 37.123 | 46.419 | 1.00 | 43.65 | C |
| ATOM | 774 | CD2 | PHE | A | 111 | 26.808 | 39.000 | 46.320 | 1.00 | 44.04 | C |
| ATOM | 775 | CE1 | PHE | A | 111 | 29.187 | 37.794 | 45.620 | 1.00 | 43.19 | C |
| ATOM | 776 | CE2 | PHE | A | 111 | 27.715 | 39.673 | 45.522 | 1.00 | 43.22 | C |
| ATOM | 777 | CZ  | PHE | A | 111 | 28.911 | 39.068 | 45.177 | 1.00 | 43.00 | C |
| ATOM | 778 | N   | GLN | A | 112 | 25.434 | 36.479 | 51.200 | 1.00 | 46.35 | N |
| ATOM | 779 | CA  | GLN | A | 112 | 24.401 | 36.052 | 52.130 | 1.00 | 46.52 | C |
| ATOM | 780 | C   | GLN | A | 112 | 23.040 | 36.638 | 51.754 | 1.00 | 46.68 | C |
| ATOM | 781 | O   | GLN | A | 112 | 22.019 | 35.995 | 51.968 | 1.00 | 46.87 | O |
| ATOM | 782 | CB  | GLN | A | 112 | 24.774 | 36.438 | 53.567 | 1.00 | 46.62 | C |
| ATOM | 783 | CG  | GLN | A | 112 | 26.201 | 36.060 | 53.998 | 1.00 | 46.96 | C |
| ATOM | 784 | CD  | GLN | A | 112 | 26.418 | 34.554 | 54.125 | 1.00 | 48.05 | C |
| ATOM | 785 | OE1 | GLN | A | 112 | 25.834 | 33.762 | 53.372 | 1.00 | 47.89 | O |
| ATOM | 786 | NE2 | GLN | A | 112 | 27.271 | 34.158 | 55.075 | 1.00 | 48.55 | N |
| ATOM | 787 | N   | ASN | A | 113 | 23.019 | 37.836 | 51.168 | 1.00 | 46.80 | N |
| ATOM | 788 | CA  | ASN | A | 113 | 21.750 | 38.463 | 50.793 | 1.00 | 46.89 | C |
| ATOM | 789 | C   | ASN | A | 113 | 21.104 | 37.951 | 49.517 | 1.00 | 47.08 | C |
| ATOM | 790 | O   | ASN | A | 113 | 20.105 | 38.521 | 49.077 | 1.00 | 47.55 | O |
| ATOM | 791 | CB  | ASN | A | 113 | 21.898 | 39.976 | 50.682 | 1.00 | 46.69 | C |
| ATOM | 792 | CG  | ASN | A | 113 | 22.258 | 40.604 | 52.001 | 1.00 | 46.91 | C |
| ATOM | 793 | OD1 | ASN | A | 113 | 22.085 | 39.982 | 53.055 | 1.00 | 46.08 | O |
| ATOM | 794 | ND2 | ASN | A | 113 | 22.767 | 41.837 | 51.962 | 1.00 | 46.59 | N |
| ATOM | 795 | N   | PHE | A | 114 | 21.651 | 36.908 | 48.903 | 1.00 | 47.08 | N |
| ATOM | 796 | CA  | PHE | A | 114 | 21.012 | 36.379 | 47.706 | 1.00 | 47.01 | C |
| ATOM | 797 | C   | PHE | A | 114 | 19.986 | 35.364 | 48.145 | 1.00 | 47.11 | C |
| ATOM | 798 | O   | PHE | A | 114 | 20.293 | 34.449 | 48.916 | 1.00 | 47.34 | O |
| ATOM | 799 | CB  | PHE | A | 114 | 21.995 | 35.713 | 46.764 | 1.00 | 46.83 | C |
| ATOM | 800 | CG  | PHE | A | 114 | 21.342 | 35.132 | 45.555 | 1.00 | 47.03 | C |
| ATOM | 801 | CD1 | PHE | A | 114 | 20.674 | 35.953 | 44.655 | 1.00 | 47.22 | C |
| ATOM | 802 | CD2 | PHE | A | 114 | 21.376 | 33.761 | 45.318 | 1.00 | 47.97 | C |
| ATOM | 803 | CE1 | PHE | A | 114 | 20.060 | 35.422 | 43.522 | 1.00 | 47.53 | C |



|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 804 | CE2 | PHE | A | 114 | 20.763 | 33.212 | 44.177 | 1.00 | 47.83 | C |
| ATOM | 805 | CZ  | PHE | A | 114 | 20.104 | 34.044 | 43.282 | 1.00 | 47.67 | C |
| ATOM | 806 | N   | LYS | A | 115 | 18.763 | 35.530 | 47.662 | 1.00 | 46.94 | N |
| ATOM | 807 | CA  | LYS | A | 115 | 17.683 | 34.628 | 48.029 | 1.00 | 46.64 | C |
| ATOM | 808 | C   | LYS | A | 115 | 17.109 | 34.063 | 46.744 | 1.00 | 46.38 | C |
| ATOM | 809 | O   | LYS | A | 115 | 16.351 | 34.744 | 46.046 | 1.00 | 46.75 | O |
| ATOM | 810 | CB  | LYS | A | 115 | 16.613 | 35.372 | 48.835 | 1.00 | 46.60 | C |
| ATOM | 811 | N   | PRO | A | 116 | 17.445 | 32.813 | 46.449 | 1.00 | 45.84 | N |
| ATOM | 812 | CA  | PRO | A | 116 | 17.079 | 32.192 | 45.165 | 1.00 | 45.70 | C |
| ATOM | 813 | C   | PRO | A | 116 | 15.576 | 32.139 | 44.937 | 1.00 | 45.44 | C |
| ATOM | 814 | O   | PRO | A | 116 | 14.827 | 31.956 | 45.892 | 1.00 | 45.46 | O |
| ATOM | 815 | CB  | PRO | A | 116 | 17.640 | 30.761 | 45.260 | 1.00 | 45.71 | C |
| ATOM | 816 | CG  | PRO | A | 116 | 18.435 | 30.689 | 46.536 | 1.00 | 45.66 | C |
| ATOM | 817 | CD  | PRO | A | 116 | 18.137 | 31.890 | 47.359 | 1.00 | 45.75 | C |
| ATOM | 818 | N   | ARG | A | 117 | 15.154 | 32.307 | 43.688 | 1.00 | 45.27 | N |
| ATOM | 819 | CA  | ARG | A | 117 | 13.742 | 32.232 | 43.332 | 1.00 | 45.16 | C |
| ATOM | 820 | C   | ARG | A | 117 | 13.291 | 30.791 | 43.104 | 1.00 | 45.12 | C |
| ATOM | 821 | O   | ARG | A | 117 | 12.096 | 30.500 | 43.207 | 1.00 | 45.48 | O |
| ATOM | 822 | CB  | ARG | A | 117 | 13.467 | 33.059 | 42.097 | 1.00 | 45.26 | C |
| ATOM | 823 | N   | SER | A | 118 | 14.238 | 29.902 | 42.796 | 1.00 | 44.78 | N |
| ATOM | 824 | CA  | SER | A | 118 | 13.944 | 28.480 | 42.594 | 1.00 | 44.60 | C |
| ATOM | 825 | C   | SER | A | 118 | 14.782 | 27.583 | 43.509 | 1.00 | 44.63 | C |
| ATOM | 826 | O   | SER | A | 118 | 15.925 | 27.921 | 43.816 | 1.00 | 45.32 | O |
| ATOM | 827 | CB  | SER | A | 118 | 14.303 | 28.072 | 41.184 | 1.00 | 44.44 | C |
| ATOM | 828 | OG  | SER | A | 118 | 15.651 | 27.624 | 41.186 | 1.00 | 44.35 | O |
| ATOM | 829 | N   | ASN | A | 119 | 14.241 | 26.428 | 43.899 | 1.00 | 44.11 | N |
| ATOM | 830 | CA  | ASN | A | 119 | 14.969 | 25.472 | 44.728 | 1.00 | 43.72 | C |
| ATOM | 831 | C   | ASN | A | 119 | 15.295 | 24.196 | 43.953 | 1.00 | 43.16 | C |
| ATOM | 832 | O   | ASN | A | 119 | 14.576 | 23.821 | 43.030 | 1.00 | 43.23 | O |
| ATOM | 833 | CB  | ASN | A | 119 | 14.147 | 25.078 | 45.955 | 1.00 | 44.03 | C |
| ATOM | 834 | CG  | ASN | A | 119 | 13.514 | 26.264 | 46.646 | 1.00 | 44.80 | C |
| ATOM | 835 | OD1 | ASN | A | 119 | 14.207 | 27.129 | 47.197 | 1.00 | 46.56 | O |
| ATOM | 836 | ND2 | ASN | A | 119 | 12.184 | 26.303 | 46.640 | 1.00 | 45.18 | N |
| ATOM | 837 | N   | ARG | A | 120 | 16.380 | 23.533 | 44.337 | 1.00 | 42.37 | N |
| ATOM | 838 | CA  | ARG | A | 120 | 16.778 | 22.278 | 43.716 | 1.00 | 41.69 | C |
| ATOM | 839 | C   | ARG | A | 120 | 16.368 | 21.162 | 44.656 | 1.00 | 41.20 | C |
| ATOM | 840 | O   | ARG | A | 120 | 16.577 | 21.267 | 45.859 | 1.00 | 41.46 | O |
| ATOM | 841 | CB  | ARG | A | 120 | 18.299 | 22.239 | 43.504 | 1.00 | 41.70 | C |
| ATOM | 842 | CG  | ARG | A | 120 | 18.827 | 21.002 | 42.754 | 1.00 | 40.96 | C |
| ATOM | 843 | CD  | ARG | A | 120 | 20.351 | 20.897 | 42.683 | 1.00 | 39.92 | C |
| ATOM | 844 | NE  | ARG | A | 120 | 21.001 | 21.327 | 43.920 | 1.00 | 39.89 | N |
| ATOM | 845 | CZ  | ARG | A | 120 | 21.337 | 20.523 | 44.921 | 1.00 | 39.57 | C |
| ATOM | 846 | NH1 | ARG | A | 120 | 21.084 | 19.217 | 44.856 | 1.00 | 39.43 | N |
| ATOM | 847 | NH2 | ARG | A | 120 | 21.930 | 21.027 | 45.998 | 1.00 | 39.06 | N |
| ATOM | 848 | N   | GLU | A | 121 | 15.769 | 20.109 | 44.115 | 1.00 | 40.44 | N |
| ATOM | 849 | CA  | GLU | A | 121 | 15.380 | 18.956 | 44.908 | 1.00 | 39.92 | C |
| ATOM | 850 | C   | GLU | A | 121 | 15.840 | 17.702 | 44.161 | 1.00 | 39.36 | C |
| ATOM | 851 | O   | GLU | A | 121 | 15.716 | 17.617 | 42.942 | 1.00 | 39.20 | O |
| ATOM | 852 | CB  | GLU | A | 121 | 13.866 | 18.950 | 45.170 | 1.00 | 39.97 | C |
| ATOM | 853 | CG  | GLU | A | 121 | 13.369 | 17.698 | 45.876 | 1.00 | 40.42 | C |
| ATOM | 854 | CD  | GLU | A | 121 | 12.136 | 17.928 | 46.731 | 1.00 | 41.22 | C |
| ATOM | 855 | OE1 | GLU | A | 121 | 12.291 | 18.365 | 47.890 | 1.00 | 41.90 | O |
| ATOM | 856 | OE2 | GLU | A | 121 | 11.016 | 17.645 | 46.259 | 1.00 | 42.21 | O |
| ATOM | 857 | N   | GLU | A | 122 | 16.414 | 16.752 | 44.889 | 1.00 | 38.78 | N |
| ATOM | 858 | CA  | GLU | A | 122 | 16.879 | 15.519 | 44.285 | 1.00 | 38.34 | C |
| ATOM | 859 | C   | GLU | A | 122 | 15.760 | 14.523 | 44.374 | 1.00 | 38.13 | C |
| ATOM | 860 | O   | GLU | A | 122 | 15.171 | 14.353 | 45.435 | 1.00 | 38.09 | O |
| ATOM | 861 | CB  | GLU | A | 122 | 18.092 | 14.989 | 45.025 | 1.00 | 38.08 | C |
| ATOM | 862 | CG  | GLU | A | 122 | 19.263 | 15.928 | 44.936 | 1.00 | 38.04 | C |
| ATOM | 863 | CD  | GLU | A | 122 | 19.581 | 16.289 | 43.497 | 1.00 | 39.25 | C |
| ATOM | 864 | OE1 | GLU | A | 122 | 19.763 | 15.364 | 42.667 | 1.00 | 38.89 | O |



|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 865 | OE2 | GLU | A | 122 | 19.627 | 17.501 | 43.183 | 1.00 | 40.06 | O |
| ATOM | 866 | N   | MET | A | 123 | 15.434 | 13.879 | 43.265 | 1.00 | 37.93 | N |
| ATOM | 867 | CA  | MET | A | 123 | 14.384 | 12.885 | 43.312 | 1.00 | 37.84 | C |
| ATOM | 868 | C   | MET | A | 123 | 14.536 | 11.819 | 42.242 | 1.00 | 37.41 | C |
| ATOM | 869 | O   | MET | A | 123 | 15.418 | 11.876 | 41.387 | 1.00 | 37.04 | O |
| ATOM | 870 | CB  | MET | A | 123 | 13.021 | 13.565 | 43.225 | 1.00 | 38.01 | C |
| ATOM | 871 | CG  | MET | A | 123 | 12.798 | 14.318 | 41.946 | 1.00 | 39.05 | C |
| ATOM | 872 | SD  | MET | A | 123 | 11.177 | 15.064 | 41.910 | 1.00 | 41.38 | S |
| ATOM | 873 | CE  | MET | A | 123 | 11.489 | 16.589 | 42.818 | 1.00 | 41.39 | C |
| ATOM | 874 | N   | LYS | A | 124 | 13.675 | 10.820 | 42.332 | 1.00 | 37.17 | N |
| ATOM | 875 | CA  | LYS | A | 124 | 13.692 | 9.715  | 41.401 | 1.00 | 36.98 | C |
| ATOM | 876 | C   | LYS | A | 124 | 12.802 | 10.098 | 40.238 | 1.00 | 36.81 | C |
| ATOM | 877 | O   | LYS | A | 124 | 11.814 | 10.813 | 40.402 | 1.00 | 36.91 | O |
| ATOM | 878 | CB  | LYS | A | 124 | 13.213 | 8.434  | 42.087 | 1.00 | 36.82 | C |
| ATOM | 879 | CG  | LYS | A | 124 | 14.081 | 7.989  | 43.281 | 1.00 | 36.79 | C |
| ATOM | 880 | CD  | LYS | A | 124 | 15.488 | 7.553  | 42.856 | 1.00 | 36.83 | C |
| ATOM | 881 | CE  | LYS | A | 124 | 16.390 | 7.206  | 44.031 | 1.00 | 36.89 | C |
| ATOM | 882 | NZ  | LYS | A | 124 | 17.822 | 7.412  | 43.680 | 1.00 | 36.99 | N |
| ATOM | 883 | N   | PHE | A | 125 | 13.145 | 9.622  | 39.056 | 1.00 | 36.49 | N |
| ATOM | 884 | CA  | PHE | A | 125 | 12.416 | 10.031 | 37.885 | 1.00 | 36.33 | C |
| ATOM | 885 | C   | PHE | A | 125 | 10.926 | 9.861  | 38.074 | 1.00 | 36.45 | C |
| ATOM | 886 | O   | PHE | A | 125 | 10.143 | 10.743 | 37.732 | 1.00 | 36.30 | O |
| ATOM | 887 | CB  | PHE | A | 125 | 12.879 | 9.270  | 36.665 | 1.00 | 36.24 | C |
| ATOM | 888 | CG  | PHE | A | 125 | 12.555 | 9.967  | 35.407 | 1.00 | 36.21 | C |
| ATOM | 889 | CD1 | PHE | A | 125 | 13.403 | 10.936 | 34.924 | 1.00 | 35.98 | C |
| ATOM | 890 | CD2 | PHE | A | 125 | 11.374 | 9.714  | 34.743 | 1.00 | 36.15 | C |
| ATOM | 891 | CE1 | PHE | A | 125 | 13.108 | 11.616 | 33.794 | 1.00 | 36.07 | C |
| ATOM | 892 | CE2 | PHE | A | 125 | 11.073 | 10.390 | 33.597 | 1.00 | 36.71 | C |
| ATOM | 893 | CZ  | PHE | A | 125 | 11.943 | 11.350 | 33.120 | 1.00 | 36.73 | C |
| ATOM | 894 | N   | HIS | A | 126 | 10.527 | 8.733  | 38.640 | 1.00 | 36.80 | N |
| ATOM | 895 | CA  | HIS | A | 126 | 9.111  | 8.492  | 38.845 | 1.00 | 36.98 | C |
| ATOM | 896 | C   | HIS | A | 126 | 8.547  | 9.560  | 39.772 | 1.00 | 37.20 | C |
| ATOM | 897 | O   | HIS | A | 126 | 7.376  | 9.923  | 39.669 | 1.00 | 37.15 | O |
| ATOM | 898 | CB  | HIS | A | 126 | 8.845  | 7.080  | 39.390 | 1.00 | 36.97 | C |
| ATOM | 899 | CG  | HIS | A | 126 | 8.990  | 6.946  | 40.877 | 1.00 | 36.62 | C |
| ATOM | 900 | ND1 | HIS | A | 126 | 7.935  | 7.115  | 41.747 | 1.00 | 35.91 | N |
| ATOM | 901 | CD2 | HIS | A | 126 | 10.058 | 6.618  | 41.644 | 1.00 | 36.38 | C |
| ATOM | 902 | CE1 | HIS | A | 126 | 8.352  | 6.921  | 42.986 | 1.00 | 35.63 | C |
| ATOM | 903 | NE2 | HIS | A | 126 | 9.636  | 6.619  | 42.951 | 1.00 | 35.43 | N |
| ATOM | 904 | N   | GLU | A | 127 | 9.383  | 10.082 | 40.663 | 1.00 | 37.34 | N |
| ATOM | 905 | CA  | GLU | A | 127 | 8.912  | 11.087 | 41.599 | 1.00 | 37.55 | C |
| ATOM | 906 | C   | GLU | A | 127 | 8.657  | 12.379 | 40.835 | 1.00 | 37.54 | C |
| ATOM | 907 | O   | GLU | A | 127 | 7.657  | 13.061 | 41.049 | 1.00 | 37.36 | O |
| ATOM | 908 | CB  | GLU | A | 127 | 9.914  | 11.308 | 42.736 | 1.00 | 37.65 | C |
| ATOM | 909 | CG  | GLU | A | 127 | 10.155 | 10.091 | 43.617 | 1.00 | 37.89 | C |
| ATOM | 910 | CD  | GLU | A | 127 | 11.113 | 10.383 | 44.764 | 1.00 | 38.14 | C |
| ATOM | 911 | OE1 | GLU | A | 127 | 12.330 | 10.531 | 44.520 | 1.00 | 37.77 | O |
| ATOM | 912 | OE2 | GLU | A | 127 | 10.649 | 10.471 | 45.917 | 1.00 | 38.86 | O |
| ATOM | 913 | N   | PHE | A | 128 | 9.557  | 12.702 | 39.920 | 1.00 | 37.65 | N |
| ATOM | 914 | CA  | PHE | A | 128 | 9.393  | 13.904 | 39.127 | 1.00 | 37.81 | C |
| ATOM | 915 | C   | PHE | A | 128 | 8.090  | 13.798 | 38.350 | 1.00 | 37.95 | C |
| ATOM | 916 | O   | PHE | A | 128 | 7.280  | 14.726 | 38.342 | 1.00 | 37.90 | O |
| ATOM | 917 | CB  | PHE | A | 128 | 10.578 | 14.061 | 38.173 | 1.00 | 37.88 | C |
| ATOM | 918 | CG  | PHE | A | 128 | 10.332 | 15.012 | 37.028 | 1.00 | 37.52 | C |
| ATOM | 919 | CD1 | PHE | A | 128 | 10.088 | 16.355 | 37.258 | 1.00 | 36.94 | C |
| ATOM | 920 | CD2 | PHE | A | 128 | 10.380 | 14.559 | 35.720 | 1.00 | 37.02 | C |
| ATOM | 921 | CE1 | PHE | A | 128 | 9.876  | 17.219 | 36.203 | 1.00 | 37.09 | C |
| ATOM | 922 | CE2 | PHE | A | 128 | 10.170 | 15.423 | 34.663 | 1.00 | 37.21 | C |
| ATOM | 923 | CZ  | PHE | A | 128 | 9.917  | 16.748 | 34.901 | 1.00 | 37.15 | C |
| ATOM | 924 | N   | VAL | A | 129 | 7.878  | 12.646 | 37.726 | 1.00 | 38.00 | N |
| ATOM | 925 | CA  | VAL | A | 129 | 6.716  | 12.454 | 36.876 | 1.00 | 38.16 | C |

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 926 | C   | VAL | A | 129 | 5.442  | 12.637 | 37.671 | 1.00 | 38.24 | C |
| ATOM | 927 | O   | VAL | A | 129 | 4.494  | 13.286 | 37.224 | 1.00 | 38.04 | O |
| ATOM | 928 | CB  | VAL | A | 129 | 6.705  | 11.050 | 36.268 | 1.00 | 38.36 | C |
| ATOM | 929 | CG1 | VAL | A | 129 | 5.398  | 10.810 | 35.508 | 1.00 | 38.41 | C |
| ATOM | 930 | CG2 | VAL | A | 129 | 7.935  | 10.841 | 35.372 | 1.00 | 38.22 | C |
| ATOM | 931 | N   | GLU | A | 130 | 5.430  | 12.038 | 38.854 | 1.00 | 38.42 | N |
| ATOM | 932 | CA  | GLU | A | 130 | 4.289  | 12.115 | 39.745 | 1.00 | 38.54 | C |
| ATOM | 933 | C   | GLU | A | 130 | 4.025  | 13.578 | 40.083 | 1.00 | 38.43 | C |
| ATOM | 934 | O   | GLU | A | 130 | 2.898  | 14.056 | 39.960 | 1.00 | 38.29 | O |
| ATOM | 935 | CB  | GLU | A | 130 | 4.547  | 11.265 | 40.997 | 1.00 | 38.69 | C |
| ATOM | 936 | CG  | GLU | A | 130 | 4.404  | 9.763  | 40.745 | 1.00 | 39.15 | C |
| ATOM | 937 | CD  | GLU | A | 130 | 5.160  | 8.897  | 41.740 | 1.00 | 39.75 | C |
| ATOM | 938 | OE1 | GLU | A | 130 | 5.551  | 9.403  | 42.815 | 1.00 | 40.08 | O |
| ATOM | 939 | OE2 | GLU | A | 130 | 5.355  | 7.697  | 41.441 | 1.00 | 40.15 | O |
| ATOM | 940 | N   | LYS | A | 131 | 5.070  | 14.299 | 40.471 | 1.00 | 38.39 | N |
| ATOM | 941 | CA  | LYS | A | 131 | 4.908  | 15.707 | 40.787 | 1.00 | 38.52 | C |
| ATOM | 942 | C   | LYS | A | 131 | 4.290  | 16.431 | 39.598 | 1.00 | 38.61 | C |
| ATOM | 943 | O   | LYS | A | 131 | 3.393  | 17.252 | 39.769 | 1.00 | 38.51 | O |
| ATOM | 944 | CB  | LYS | A | 131 | 6.240  | 16.356 | 41.149 | 1.00 | 38.58 | C |
| ATOM | 945 | CG  | LYS | A | 131 | 6.440  | 16.666 | 42.625 | 1.00 | 38.76 | C |
| ATOM | 946 | CD  | LYS | A | 131 | 7.045  | 18.060 | 42.753 | 1.00 | 39.73 | C |
| ATOM | 947 | CE  | LYS | A | 131 | 7.756  | 18.316 | 44.070 | 1.00 | 40.49 | C |
| ATOM | 948 | NZ  | LYS | A | 131 | 8.117  | 19.772 | 44.197 | 1.00 | 40.68 | N |
| ATOM | 949 | N   | LEU | A | 132 | 4.764  | 16.136 | 38.391 | 1.00 | 38.84 | N |
| ATOM | 950 | CA  | LEU | A | 132 | 4.196  | 16.771 | 37.208 | 1.00 | 39.00 | C |
| ATOM | 951 | C   | LEU | A | 132 | 2.726  | 16.429 | 37.113 | 1.00 | 39.11 | C |
| ATOM | 952 | O   | LEU | A | 132 | 1.903  | 17.287 | 36.810 | 1.00 | 39.20 | O |
| ATOM | 953 | CB  | LEU | A | 132 | 4.894  | 16.328 | 35.932 | 1.00 | 38.96 | C |
| ATOM | 954 | CG  | LEU | A | 132 | 6.287  | 16.899 | 35.723 | 1.00 | 39.44 | C |
| ATOM | 955 | CD1 | LEU | A | 132 | 6.870  | 16.389 | 34.429 | 1.00 | 39.81 | C |
| ATOM | 956 | CD2 | LEU | A | 132 | 6.261  | 18.421 | 35.709 | 1.00 | 40.07 | C |
| ATOM | 957 | N   | GLN | A | 133 | 2.396  | 15.170 | 37.367 | 1.00 | 39.22 | N |
| ATOM | 958 | CA  | GLN | A | 133 | 1.005  | 14.758 | 37.335 | 1.00 | 39.38 | C |
| ATOM | 959 | C   | GLN | A | 133 | 0.172  | 15.523 | 38.370 | 1.00 | 39.57 | C |
| ATOM | 960 | O   | GLN | A | 133 | -0.893 | 16.034 | 38.029 | 1.00 | 39.48 | O |
| ATOM | 961 | CB  | GLN | A | 133 | 0.874  | 13.250 | 37.536 | 1.00 | 39.22 | C |
| ATOM | 962 | N   | ASP | A | 134 | 0.656  | 15.631 | 39.611 | 1.00 | 39.91 | N |
| ATOM | 963 | CA  | ASP | A | 134 | -0.129 | 16.279 | 40.677 | 1.00 | 40.29 | C |
| ATOM | 964 | C   | ASP | A | 134 | -0.437 | 17.732 | 40.379 | 1.00 | 40.17 | C |
| ATOM | 965 | O   | ASP | A | 134 | -1.543 | 18.211 | 40.623 | 1.00 | 40.02 | O |
| ATOM | 966 | CB  | ASP | A | 134 | 0.564  | 16.198 | 42.041 | 1.00 | 40.57 | C |
| ATOM | 967 | CG  | ASP | A | 134 | -0.348 | 16.660 | 43.182 | 1.00 | 41.99 | C |
| ATOM | 968 | OD1 | ASP | A | 134 | -1.301 | 17.421 | 42.910 | 1.00 | 43.76 | O |
| ATOM | 969 | OD2 | ASP | A | 134 | -0.212 | 16.312 | 44.378 | 1.00 | 44.05 | O |
| ATOM | 970 | N   | ILE | A | 135 | 0.545  | 18.438 | 39.846 | 1.00 | 40.17 | N |
| ATOM | 971 | CA  | ILE | A | 135 | 0.350  | 19.836 | 39.556 | 1.00 | 40.10 | C |
| ATOM | 972 | C   | ILE | A | 135 | -0.719 | 19.973 | 38.500 | 1.00 | 40.10 | C |
| ATOM | 973 | O   | ILE | A | 135 | -1.648 | 20.759 | 38.652 | 1.00 | 40.26 | O |
| ATOM | 974 | CB  | ILE | A | 135 | 1.639  | 20.455 | 39.085 | 1.00 | 40.10 | C |
| ATOM | 975 | CG1 | ILE | A | 135 | 2.612  | 20.560 | 40.261 | 1.00 | 40.11 | C |
| ATOM | 976 | CG2 | ILE | A | 135 | 1.358  | 21.817 | 38.507 | 1.00 | 40.22 | C |
| ATOM | 977 | CD1 | ILE | A | 135 | 4.056  | 20.688 | 39.842 | 1.00 | 40.17 | C |
| ATOM | 978 | N   | GLN | A | 136 | -0.596 | 19.198 | 37.431 | 1.00 | 40.02 | N |
| ATOM | 979 | CA  | GLN | A | 136 | -1.586 | 19.248 | 36.376 | 1.00 | 39.96 | C |
| ATOM | 980 | C   | GLN | A | 136 | -2.956 | 19.094 | 37.000 | 1.00 | 39.99 | C |
| ATOM | 981 | O   | GLN | A | 136 | -3.795 | 19.991 | 36.921 | 1.00 | 39.86 | O |
| ATOM | 982 | CB  | GLN | A | 136 | -1.350 | 18.144 | 35.361 | 1.00 | 40.00 | C |
| ATOM | 983 | N   | GLN | A | 137 | -3.158 | 17.972 | 37.679 | 1.00 | 40.18 | N |
| ATOM | 984 | CA  | GLN | A | 137 | -4.486 | 17.630 | 38.164 | 1.00 | 40.31 | C |
| ATOM | 985 | C   | GLN | A | 137 | -4.995 | 18.683 | 39.114 | 1.00 | 40.45 | C |
| ATOM | 986 | O   | GLN | A | 137 | -6.170 | 19.046 | 39.068 | 1.00 | 40.75 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 987  | CB  | GLN | A | 137 | -4.502 | 16.247 | 38.829 | 1.00 | 40.24 | C |
| ATOM | 988  | N   | ARG | A | 138 | -4.116 | 19.200 | 39.959 | 1.00 | 40.45 | N |
| ATOM | 989  | CA  | ARG | A | 138 | -4.560 | 20.159 | 40.956 | 1.00 | 40.45 | C |
| ATOM | 990  | C   | ARG | A | 138 | -4.568 | 21.588 | 40.419 | 1.00 | 40.54 | C |
| ATOM | 991  | O   | ARG | A | 138 | -4.678 | 22.541 | 41.188 | 1.00 | 40.67 | O |
| ATOM | 992  | CB  | ARG | A | 138 | -3.692 | 20.069 | 42.207 | 1.00 | 40.43 | C |
| ATOM | 993  | CG  | ARG | A | 138 | -2.399 | 20.868 | 42.161 | 1.00 | 40.03 | C |
| ATOM | 994  | CD  | ARG | A | 138 | -1.541 | 20.546 | 43.346 | 1.00 | 39.94 | C |
| ATOM | 995  | NE  | ARG | A | 138 | -0.431 | 21.458 | 43.580 | 1.00 | 39.71 | N |
| ATOM | 996  | CZ  | ARG | A | 138 | 0.842  | 21.098 | 43.498 | 1.00 | 40.13 | C |
| ATOM | 997  | NH1 | ARG | A | 138 | 1.164  | 19.857 | 43.150 | 1.00 | 40.53 | N |
| ATOM | 998  | NH2 | ARG | A | 138 | 1.800  | 21.978 | 43.747 | 1.00 | 40.33 | N |
| ATOM | 999  | N   | GLY | A | 139 | -4.471 | 21.742 | 39.102 | 1.00 | 40.47 | N |
| ATOM | 1000 | CA  | GLY | A | 139 | -4.418 | 23.066 | 38.508 | 1.00 | 40.46 | C |
| ATOM | 1001 | C   | GLY | A | 139 | -3.432 | 24.021 | 39.176 | 1.00 | 40.45 | C |
| ATOM | 1002 | O   | GLY | A | 139 | -3.616 | 25.235 | 39.110 | 1.00 | 40.46 | O |
| ATOM | 1003 | N   | GLY | A | 140 | -2.370 | 23.490 | 39.780 | 1.00 | 40.47 | N |
| ATOM | 1004 | CA  | GLY | A | 140 | -1.425 | 24.314 | 40.519 | 1.00 | 40.45 | C |
| ATOM | 1005 | C   | GLY | A | 140 | -0.695 | 25.272 | 39.602 | 1.00 | 40.40 | C |
| ATOM | 1006 | O   | GLY | A | 140 | -0.784 | 25.116 | 38.383 | 1.00 | 40.79 | O |
| ATOM | 1007 | N   | GLU | A | 141 | -0.015 | 26.273 | 40.167 | 1.00 | 40.10 | N |
| ATOM | 1008 | CA  | GLU | A | 141 | 0.807  | 27.195 | 39.371 | 1.00 | 40.01 | C |
| ATOM | 1009 | C   | GLU | A | 141 | 2.305  | 26.854 | 39.458 | 1.00 | 39.64 | C |
| ATOM | 1010 | O   | GLU | A | 141 | 3.112  | 27.386 | 38.692 | 1.00 | 39.52 | O |
| ATOM | 1011 | CB  | GLU | A | 141 | 0.589  | 28.660 | 39.796 | 1.00 | 40.20 | C |
| ATOM | 1012 | CG  | GLU | A | 141 | -0.711 | 29.298 | 39.315 | 1.00 | 41.00 | C |
| ATOM | 1013 | CD  | GLU | A | 141 | -0.845 | 29.307 | 37.800 | 1.00 | 42.10 | C |
| ATOM | 1014 | OE1 | GLU | A | 141 | 0.194  | 29.181 | 37.113 | 1.00 | 41.99 | O |
| ATOM | 1015 | OE2 | GLU | A | 141 | -1.990 | 29.437 | 37.300 | 1.00 | 43.15 | O |
| ATOM | 1016 | N   | GLU | A | 142 | 2.676  | 25.977 | 40.392 | 1.00 | 39.25 | N |
| ATOM | 1017 | CA  | GLU | A | 142 | 4.075  | 25.589 | 40.563 | 1.00 | 38.95 | C |
| ATOM | 1018 | C   | GLU | A | 142 | 4.613  | 25.162 | 39.210 | 1.00 | 38.74 | C |
| ATOM | 1019 | O   | GLU | A | 142 | 3.859  | 24.694 | 38.351 | 1.00 | 38.77 | O |
| ATOM | 1020 | CB  | GLU | A | 142 | 4.220  | 24.433 | 41.577 | 1.00 | 38.95 | C |
| ATOM | 1021 | CG  | GLU | A | 142 | 5.658  | 24.138 | 42.019 | 1.00 | 38.90 | C |
| ATOM | 1022 | CD  | GLU | A | 142 | 5.797  | 22.950 | 42.971 | 1.00 | 38.93 | C |
| ATOM | 1023 | OE1 | GLU | A | 142 | 4.836  | 22.164 | 43.130 | 1.00 | 39.58 | O |
| ATOM | 1024 | OE2 | GLU | A | 142 | 6.888  | 22.799 | 43.565 | 1.00 | 38.74 | O |
| ATOM | 1025 | N   | ARG | A | 143 | 5.914  | 25.332 | 39.020 | 1.00 | 38.39 | N |
| ATOM | 1026 | CA  | ARG | A | 143 | 6.569  | 24.908 | 37.796 | 1.00 | 38.25 | C |
| ATOM | 1027 | C   | ARG | A | 143 | 7.809  | 24.122 | 38.122 | 1.00 | 38.14 | C |
| ATOM | 1028 | O   | ARG | A | 143 | 8.512  | 24.450 | 39.078 | 1.00 | 38.46 | O |
| ATOM | 1029 | CB  | ARG | A | 143 | 7.046  | 26.107 | 37.003 | 1.00 | 38.26 | C |
| ATOM | 1030 | CG  | ARG | A | 143 | 5.986  | 26.945 | 36.398 | 1.00 | 37.89 | C |
| ATOM | 1031 | CD  | ARG | A | 143 | 6.602  | 28.026 | 35.555 | 1.00 | 37.35 | C |
| ATOM | 1032 | NE  | ARG | A | 143 | 5.610  | 28.814 | 34.849 | 1.00 | 36.66 | N |
| ATOM | 1033 | CZ  | ARG | A | 143 | 5.316  | 28.668 | 33.573 | 1.00 | 36.40 | C |
| ATOM | 1034 | NH1 | ARG | A | 143 | 5.933  | 27.755 | 32.831 | 1.00 | 36.41 | N |
| ATOM | 1035 | NH2 | ARG | A | 143 | 4.397  | 29.443 | 33.034 | 1.00 | 37.02 | N |
| ATOM | 1036 | N   | LEU | A | 144 | 8.116  | 23.124 | 37.304 | 1.00 | 37.71 | N |
| ATOM | 1037 | CA  | LEU | A | 144 | 9.319  | 22.349 | 37.517 | 1.00 | 37.57 | C |
| ATOM | 1038 | C   | LEU | A | 144 | 10.181 | 22.319 | 36.294 | 1.00 | 37.33 | C |
| ATOM | 1039 | O   | LEU | A | 144 | 9.710  | 22.466 | 35.165 | 1.00 | 37.31 | O |
| ATOM | 1040 | CB  | LEU | A | 144 | 8.979  | 20.909 | 37.858 | 1.00 | 37.69 | C |
| ATOM | 1041 | CG  | LEU | A | 144 | 7.981  | 20.736 | 38.993 | 1.00 | 38.31 | C |
| ATOM | 1042 | CD1 | LEU | A | 144 | 7.612  | 19.255 | 39.165 | 1.00 | 39.02 | C |
| ATOM | 1043 | CD2 | LEU | A | 144 | 8.551  | 21.327 | 40.263 | 1.00 | 37.91 | C |
| ATOM | 1044 | N   | TYR | A | 145 | 11.460 | 22.098 | 36.528 | 1.00 | 37.01 | N |
| ATOM | 1045 | CA  | TYR | A | 145 | 12.379 | 21.922 | 35.437 | 1.00 | 36.87 | C |
| ATOM | 1046 | C   | TYR | A | 145 | 13.397 | 20.886 | 35.871 | 1.00 | 36.85 | C |
| ATOM | 1047 | O   | TYR | A | 145 | 14.146 | 21.093 | 36.819 | 1.00 | 36.51 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1048 | CB  | TYR | A | 145 | 13.043 | 23.255 | 35.110 | 1.00 | 36.92 | C |
| ATOM | 1049 | CG  | TYR | A | 145 | 13.505 | 23.446 | 33.686 | 1.00 | 36.38 | C |
| ATOM | 1050 | CD1 | TYR | A | 145 | 13.845 | 22.383 | 32.875 | 1.00 | 36.31 | C |
| ATOM | 1051 | CD2 | TYR | A | 145 | 13.619 | 24.716 | 33.163 | 1.00 | 36.28 | C |
| ATOM | 1052 | CE1 | TYR | A | 145 | 14.278 | 22.590 | 31.582 | 1.00 | 36.21 | C |
| ATOM | 1053 | CE2 | TYR | A | 145 | 14.047 | 24.923 | 31.880 | 1.00 | 35.94 | C |
| ATOM | 1054 | CZ  | TYR | A | 145 | 14.374 | 23.862 | 31.093 | 1.00 | 35.54 | C |
| ATOM | 1055 | OH  | TYR | A | 145 | 14.789 | 24.081 | 29.799 | 1.00 | 36.13 | O |
| ATOM | 1056 | N   | LEU | A | 146 | 13.378 | 19.736 | 35.218 | 1.00 | 37.06 | N |
| ATOM | 1057 | CA  | LEU | A | 146 | 14.396 | 18.742 | 35.477 | 1.00 | 37.49 | C |
| ATOM | 1058 | C   | LEU | A | 146 | 15.628 | 19.029 | 34.629 | 1.00 | 37.55 | C |
| ATOM | 1059 | O   | LEU | A | 146 | 15.532 | 19.241 | 33.427 | 1.00 | 37.31 | O |
| ATOM | 1060 | CB  | LEU | A | 146 | 13.877 | 17.341 | 35.173 | 1.00 | 37.69 | C |
| ATOM | 1061 | CG  | LEU | A | 146 | 14.919 | 16.233 | 35.349 | 1.00 | 37.95 | C |
| ATOM | 1062 | CD1 | LEU | A | 146 | 14.234 | 14.916 | 35.567 | 1.00 | 37.66 | C |
| ATOM | 1063 | CD2 | LEU | A | 146 | 15.849 | 16.133 | 34.151 | 1.00 | 39.00 | C |
| ATOM | 1064 | N   | GLN | A | 147 | 16.786 | 18.993 | 35.269 | 1.00 | 37.84 | N |
| ATOM | 1065 | CA  | GLN | A | 147 | 18.053 | 19.259 | 34.617 | 1.00 | 38.09 | C |
| ATOM | 1066 | C   | GLN | A | 147 | 19.088 | 18.397 | 35.306 | 1.00 | 37.92 | C |
| ATOM | 1067 | O   | GLN | A | 147 | 19.453 | 18.661 | 36.443 | 1.00 | 37.87 | O |
| ATOM | 1068 | CB  | GLN | A | 147 | 18.421 | 20.725 | 34.773 | 1.00 | 38.37 | C |
| ATOM | 1069 | CG  | GLN | A | 147 | 17.331 | 21.686 | 34.362 | 1.00 | 39.01 | C |
| ATOM | 1070 | CD  | GLN | A | 147 | 17.867 | 23.064 | 34.191 | 1.00 | 39.92 | C |
| ATOM | 1071 | OE1 | GLN | A | 147 | 17.149 | 23.955 | 33.772 | 1.00 | 42.51 | O |
| ATOM | 1072 | NE2 | GLN | A | 147 | 19.137 | 23.253 | 34.520 | 1.00 | 40.24 | N |
| ATOM | 1073 | N   | GLN | A | 148 | 19.576 | 17.385 | 34.601 | 1.00 | 37.81 | N |
| ATOM | 1074 | CA  | GLN | A | 148 | 20.433 | 16.377 | 35.196 | 1.00 | 37.57 | C |
| ATOM | 1075 | C   | GLN | A | 148 | 21.325 | 15.744 | 34.176 | 1.00 | 37.68 | C |
| ATOM | 1076 | O   | GLN | A | 148 | 20.876 | 15.266 | 33.146 | 1.00 | 37.30 | O |
| ATOM | 1077 | CB  | GLN | A | 148 | 19.576 | 15.261 | 35.773 | 1.00 | 37.61 | C |
| ATOM | 1078 | CG  | GLN | A | 148 | 20.336 | 13.971 | 36.068 | 1.00 | 36.79 | C |
| ATOM | 1079 | CD  | GLN | A | 148 | 21.398 | 14.159 | 37.117 | 1.00 | 35.97 | C |
| ATOM | 1080 | OE1 | GLN | A | 148 | 21.162 | 14.814 | 38.135 | 1.00 | 35.11 | O |
| ATOM | 1081 | NE2 | GLN | A | 148 | 22.577 | 13.593 | 36.875 | 1.00 | 35.03 | N |
| ATOM | 1082 | N   | THR | A | 149 | 22.596 | 15.698 | 34.503 | 1.00 | 38.15 | N |
| ATOM | 1083 | CA  | THR | A | 149 | 23.574 | 15.130 | 33.622 | 1.00 | 38.57 | C |
| ATOM | 1084 | C   | THR | A | 149 | 23.354 | 13.647 | 33.506 | 1.00 | 38.68 | C |
| ATOM | 1085 | O   | THR | A | 149 | 23.154 | 12.973 | 34.509 | 1.00 | 39.07 | O |
| ATOM | 1086 | CB  | THR | A | 149 | 24.936 | 15.410 | 34.214 | 1.00 | 38.75 | C |
| ATOM | 1087 | OG1 | THR | A | 149 | 25.206 | 16.807 | 34.088 | 1.00 | 38.86 | O |
| ATOM | 1088 | CG2 | THR | A | 149 | 26.036 | 14.759 | 33.418 | 1.00 | 39.39 | C |
| ATOM | 1089 | N   | LEU | A | 150 | 23.393 | 13.144 | 32.279 | 1.00 | 38.87 | N |
| ATOM | 1090 | CA  | LEU | A | 150 | 23.259 | 11.722 | 32.021 | 1.00 | 39.24 | C |
| ATOM | 1091 | C   | LEU | A | 150 | 24.498 | 10.979 | 32.507 | 1.00 | 39.20 | C |
| ATOM | 1092 | O   | LEU | A | 150 | 25.602 | 11.317 | 32.101 | 1.00 | 39.20 | O |
| ATOM | 1093 | CB  | LEU | A | 150 | 23.146 | 11.465 | 30.519 | 1.00 | 39.46 | C |
| ATOM | 1094 | CG  | LEU | A | 150 | 21.938 | 11.942 | 29.722 | 1.00 | 40.52 | C |
| ATOM | 1095 | CD1 | LEU | A | 150 | 22.077 | 11.563 | 28.237 | 1.00 | 41.06 | C |
| ATOM | 1096 | CD2 | LEU | A | 150 | 20.712 | 11.308 | 30.303 | 1.00 | 41.66 | C |
| ATOM | 1097 | N   | ASN | A | 151 | 24.315 | 9.960  | 33.343 | 1.00 | 39.19 | N |
| ATOM | 1098 | CA  | ASN | A | 151 | 25.436 | 9.171  | 33.861 | 1.00 | 39.46 | C |
| ATOM | 1099 | C   | ASN | A | 151 | 25.193 | 7.642  | 33.883 | 1.00 | 39.43 | C |
| ATOM | 1100 | O   | ASN | A | 151 | 24.198 | 7.162  | 33.333 | 1.00 | 39.15 | O |
| ATOM | 1101 | CB  | ASN | A | 151 | 25.731 | 9.652  | 35.265 | 1.00 | 39.54 | C |
| ATOM | 1102 | CG  | ASN | A | 151 | 24.511 | 9.588  | 36.150 | 1.00 | 40.08 | C |
| ATOM | 1103 | OD1 | ASN | A | 151 | 23.874 | 8.533  | 36.283 | 1.00 | 39.68 | O |
| ATOM | 1104 | ND2 | ASN | A | 151 | 24.158 | 10.725 | 36.751 | 1.00 | 40.83 | N |
| ATOM | 1105 | N   | ASP | A | 152 | 26.075 | 6.892  | 34.556 | 1.00 | 39.43 | N |
| ATOM | 1106 | CA  | ASP | A | 152 | 26.025 | 5.413  | 34.543 | 1.00 | 39.58 | C |
| ATOM | 1107 | C   | ASP | A | 152 | 24.761 | 4.787  | 35.083 | 1.00 | 39.17 | C |
| ATOM | 1108 | O   | ASP | A | 152 | 24.477 | 3.634  | 34.776 | 1.00 | 39.29 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1109 | CB  | ASP | A | 152 | 27.138 | 4.756  | 35.385 | 1.00 | 39.92 | C |
| ATOM | 1110 | CG  | ASP | A | 152 | 28.489 | 5.382  | 35.198 | 1.00 | 41.53 | C |
| ATOM | 1111 | OD1 | ASP | A | 152 | 28.722 | 6.005  | 34.134 | 1.00 | 45.10 | O |
| ATOM | 1112 | OD2 | ASP | A | 152 | 29.378 | 5.294  | 36.076 | 1.00 | 42.02 | O |
| ATOM | 1113 | N   | THR | A | 153 | 24.008 | 5.493  | 35.909 | 1.00 | 38.78 | N |
| ATOM | 1114 | CA  | THR | A | 153 | 22.881 | 4.830  | 36.542 | 1.00 | 38.50 | C |
| ATOM | 1115 | C   | THR | A | 153 | 21.757 | 4.573  | 35.573 | 1.00 | 38.26 | C |
| ATOM | 1116 | O   | THR | A | 153 | 20.842 | 3.838  | 35.882 | 1.00 | 38.29 | O |
| ATOM | 1117 | CB  | THR | A | 153 | 22.329 | 5.624  | 37.733 | 1.00 | 38.46 | C |
| ATOM | 1118 | OG1 | THR | A | 153 | 21.622 | 6.780  | 37.269 | 1.00 | 39.25 | O |
| ATOM | 1119 | CG2 | THR | A | 153 | 23.445 | 6.161  | 38.611 | 1.00 | 38.28 | C |
| ATOM | 1120 | N   | VAL | A | 154 | 21.804 | 5.165  | 34.396 | 1.00 | 38.28 | N |
| ATOM | 1121 | CA  | VAL | A | 154 | 20.687 | 4.977  | 33.491 | 1.00 | 38.29 | C |
| ATOM | 1122 | C   | VAL | A | 154 | 20.602 | 3.530  | 33.067 | 1.00 | 38.17 | C |
| ATOM | 1123 | O   | VAL | A | 154 | 21.597 | 2.805  | 33.092 | 1.00 | 38.10 | O |
| ATOM | 1124 | CB  | VAL | A | 154 | 20.786 | 5.838  | 32.251 | 1.00 | 38.15 | C |
| ATOM | 1125 | CG1 | VAL | A | 154 | 20.815 | 7.291  | 32.649 | 1.00 | 38.22 | C |
| ATOM | 1126 | CG2 | VAL | A | 154 | 22.007 | 5.437  | 31.443 | 1.00 | 38.40 | C |
| ATOM | 1127 | N   | GLY | A | 155 | 19.395 | 3.132  | 32.681 | 1.00 | 38.05 | N |
| ATOM | 1128 | CA  | GLY | A | 155 | 19.114 | 1.779  | 32.258 | 1.00 | 38.07 | C |
| ATOM | 1129 | C   | GLY | A | 155 | 19.609 | 1.358  | 30.894 | 1.00 | 38.17 | C |
| ATOM | 1130 | O   | GLY | A | 155 | 20.092 | 2.153  | 30.081 | 1.00 | 38.44 | O |
| ATOM | 1131 | N   | ARG | A | 156 | 19.417 | 0.073  | 30.642 | 1.00 | 38.16 | N |
| ATOM | 1132 | CA  | ARG | A | 156 | 19.932 | -0.588 | 29.461 | 1.00 | 38.16 | C |
| ATOM | 1133 | C   | ARG | A | 156 | 19.414 | 0.065  | 28.210 | 1.00 | 38.01 | C |
| ATOM | 1134 | O   | ARG | A | 156 | 20.185 | 0.490  | 27.346 | 1.00 | 38.04 | O |
| ATOM | 1135 | CB  | ARG | A | 156 | 19.554 | -2.080 | 29.489 | 1.00 | 38.18 | C |
| ATOM | 1136 | N   | LYS | A | 157 | 18.102 | 0.178  | 28.118 | 1.00 | 37.83 | N |
| ATOM | 1137 | CA  | LYS | A | 157 | 17.545 | 0.713  | 26.905 | 1.00 | 37.67 | C |
| ATOM | 1138 | C   | LYS | A | 157 | 18.144 | 2.092  | 26.679 | 1.00 | 37.77 | C |
| ATOM | 1139 | O   | LYS | A | 157 | 18.579 | 2.386  | 25.571 | 1.00 | 37.84 | O |
| ATOM | 1140 | CB  | LYS | A | 157 | 16.014 | 0.725  | 26.936 | 1.00 | 37.62 | C |
| ATOM | 1141 | CG  | LYS | A | 157 | 15.379 | -0.624 | 26.550 | 1.00 | 36.92 | C |
| ATOM | 1142 | N   | ILE | A | 158 | 18.247 | 2.911  | 27.728 | 1.00 | 37.82 | N |
| ATOM | 1143 | CA  | ILE | A | 158 | 18.699 | 4.287  | 27.526 | 1.00 | 37.81 | C |
| ATOM | 1144 | C   | ILE | A | 158 | 20.096 | 4.252  | 27.008 | 1.00 | 37.78 | C |
| ATOM | 1145 | O   | ILE | A | 158 | 20.440 | 4.942  | 26.058 | 1.00 | 37.52 | O |
| ATOM | 1146 | CB  | ILE | A | 158 | 18.666 | 5.109  | 28.802 | 1.00 | 37.90 | C |
| ATOM | 1147 | CG1 | ILE | A | 158 | 17.233 | 5.283  | 29.280 | 1.00 | 37.87 | C |
| ATOM | 1148 | CG2 | ILE | A | 158 | 19.281 | 6.477  | 28.538 | 1.00 | 37.57 | C |
| ATOM | 1149 | CD1 | ILE | A | 158 | 16.383 | 6.034  | 28.318 | 1.00 | 37.95 | C |
| ATOM | 1150 | N   | VAL | A | 159 | 20.899 | 3.418  | 27.637 | 1.00 | 37.89 | N |
| ATOM | 1151 | CA  | VAL | A | 159 | 22.263 | 3.265  | 27.211 | 1.00 | 38.06 | C |
| ATOM | 1152 | C   | VAL | A | 159 | 22.255 | 2.906  | 25.725 | 1.00 | 38.07 | C |
| ATOM | 1153 | O   | VAL | A | 159 | 23.025 | 3.462  | 24.955 | 1.00 | 37.93 | O |
| ATOM | 1154 | CB  | VAL | A | 159 | 22.987 | 2.196  | 28.039 | 1.00 | 38.12 | C |
| ATOM | 1155 | CG1 | VAL | A | 159 | 24.208 | 1.740  | 27.315 | 1.00 | 38.65 | C |
| ATOM | 1156 | CG2 | VAL | A | 159 | 23.368 | 2.734  | 29.410 | 1.00 | 37.65 | C |
| ATOM | 1157 | N   | MET | A | 160 | 21.385 | 1.984  | 25.318 | 1.00 | 38.30 | N |
| ATOM | 1158 | CA  | MET | A | 160 | 21.264 | 1.658  | 23.894 | 1.00 | 38.71 | C |
| ATOM | 1159 | C   | MET | A | 160 | 21.024 | 2.923  | 23.084 | 1.00 | 38.35 | C |
| ATOM | 1160 | O   | MET | A | 160 | 21.742 | 3.219  | 22.137 | 1.00 | 38.42 | O |
| ATOM | 1161 | CB  | MET | A | 160 | 20.115 | 0.682  | 23.636 | 1.00 | 38.93 | C |
| ATOM | 1162 | CG  | MET | A | 160 | 20.431 | -0.690 | 24.087 | 1.00 | 40.64 | C |
| ATOM | 1163 | SD  | MET | A | 160 | 21.840 | -1.293 | 23.180 | 1.00 | 44.02 | S |
| ATOM | 1164 | CE  | MET | A | 160 | 20.982 | -1.709 | 21.617 | 1.00 | 44.00 | C |
| ATOM | 1165 | N   | ASP | A | 161 | 19.997 | 3.665  | 23.458 | 1.00 | 37.94 | N |
| ATOM | 1166 | CA  | ASP | A | 161 | 19.702 | 4.902  | 22.773 | 1.00 | 37.82 | C |
| ATOM | 1167 | C   | ASP | A | 161 | 20.955 | 5.788  | 22.684 | 1.00 | 37.50 | C |
| ATOM | 1168 | O   | ASP | A | 161 | 21.395 | 6.154  | 21.596 | 1.00 | 37.66 | O |
| ATOM | 1169 | CB  | ASP | A | 161 | 18.591 | 5.650  | 23.511 | 1.00 | 37.84 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1170 | CG  | ASP | A | 161 | 17.274 | 4.908  | 23.501 | 1.00 | 37.82 | C |
| ATOM | 1171 | OD1 | ASP | A | 161 | 17.082 | 4.020  | 22.646 | 1.00 | 37.72 | O |
| ATOM | 1172 | OD2 | ASP | A | 161 | 16.366 | 5.155  | 24.320 | 1.00 | 38.41 | O |
| ATOM | 1173 | N   | PHE | A | 162 | 21.539 | 6.100  | 23.836 | 1.00 | 36.93 | N |
| ATOM | 1174 | CA  | PHE | A | 162 | 22.672 | 7.020  | 23.919 | 1.00 | 36.54 | C |
| ATOM | 1175 | C   | PHE | A | 162 | 23.760 | 6.604  | 22.960 | 1.00 | 36.03 | C |
| ATOM | 1176 | O   | PHE | A | 162 | 24.375 | 7.446  | 22.304 | 1.00 | 36.06 | O |
| ATOM | 1177 | CB  | PHE | A | 162 | 23.201 | 7.063  | 25.364 | 1.00 | 36.52 | C |
| ATOM | 1178 | CG  | PHE | A | 162 | 24.386 | 7.974  | 25.576 | 1.00 | 36.64 | C |
| ATOM | 1179 | CD1 | PHE | A | 162 | 24.209 | 9.319  | 25.871 | 1.00 | 36.67 | C |
| ATOM | 1180 | CD2 | PHE | A | 162 | 25.682 | 7.467  | 25.540 | 1.00 | 37.81 | C |
| ATOM | 1181 | CE1 | PHE | A | 162 | 25.299 | 10.155 | 26.081 | 1.00 | 36.91 | C |
| ATOM | 1182 | CE2 | PHE | A | 162 | 26.787 | 8.300  | 25.764 | 1.00 | 37.75 | C |
| ATOM | 1183 | CZ  | PHE | A | 162 | 26.592 | 9.640  | 26.029 | 1.00 | 37.82 | C |
| ATOM | 1184 | N   | LEU | A | 163 | 23.976 | 5.297  | 22.878 | 1.00 | 35.38 | N |
| ATOM | 1185 | CA  | LEU | A | 163 | 24.998 | 4.730  | 22.023 | 1.00 | 34.93 | C |
| ATOM | 1186 | C   | LEU | A | 163 | 24.635 | 4.948  | 20.591 | 1.00 | 34.41 | C |
| ATOM | 1187 | O   | LEU | A | 163 | 25.502 | 5.067  | 19.732 | 1.00 | 34.36 | O |
| ATOM | 1188 | CB  | LEU | A | 163 | 25.111 | 3.239  | 22.272 | 1.00 | 35.05 | C |
| ATOM | 1189 | CG  | LEU | A | 163 | 25.977 | 2.932  | 23.473 | 1.00 | 35.25 | C |
| ATOM | 1190 | CD1 | LEU | A | 163 | 25.944 | 1.471  | 23.684 | 1.00 | 36.00 | C |
| ATOM | 1191 | CD2 | LEU | A | 163 | 27.404 | 3.425  | 23.270 | 1.00 | 35.64 | C |
| ATOM | 1192 | N   | GLY | A | 164 | 23.336 | 4.977  | 20.338 | 1.00 | 33.85 | N |
| ATOM | 1193 | CA  | GLY | A | 164 | 22.832 | 5.230  | 19.009 | 1.00 | 33.55 | C |
| ATOM | 1194 | C   | GLY | A | 164 | 22.874 | 6.682  | 18.548 | 1.00 | 33.11 | C |
| ATOM | 1195 | O   | GLY | A | 164 | 22.361 | 6.977  | 17.471 | 1.00 | 33.36 | O |
| ATOM | 1196 | N   | PHE | A | 165 | 23.443 | 7.589  | 19.341 | 1.00 | 32.16 | N |
| ATOM | 1197 | CA  | PHE | A | 165 | 23.593 | 8.964  | 18.894 | 1.00 | 31.85 | C |
| ATOM | 1198 | C   | PHE | A | 165 | 24.628 | 8.972  | 17.752 | 1.00 | 30.93 | C |
| ATOM | 1199 | O   | PHE | A | 165 | 25.413 | 8.063  | 17.650 | 1.00 | 30.67 | O |
| ATOM | 1200 | CB  | PHE | A | 165 | 24.028 | 9.883  | 20.055 | 1.00 | 32.06 | C |
| ATOM | 1201 | CG  | PHE | A | 165 | 22.989 | 10.052 | 21.160 | 1.00 | 32.55 | C |
| ATOM | 1202 | CD1 | PHE | A | 165 | 21.734 | 9.478  | 21.081 | 1.00 | 33.69 | C |
| ATOM | 1203 | CD2 | PHE | A | 165 | 23.293 | 10.786 | 22.289 | 1.00 | 32.64 | C |
| ATOM | 1204 | CE1 | PHE | A | 165 | 20.817 | 9.646  | 22.106 | 1.00 | 33.39 | C |
| ATOM | 1205 | CE2 | PHE | A | 165 | 22.380 | 10.948 | 23.308 | 1.00 | 32.11 | C |
| ATOM | 1206 | CZ  | PHE | A | 165 | 21.150 | 10.380 | 23.218 | 1.00 | 32.69 | C |
| ATOM | 1207 | N   | ASN | A | 166 | 24.600 | 9.977  | 16.881 | 1.00 | 30.43 | N |
| ATOM | 1208 | CA  | ASN | A | 166 | 25.552 | 10.106 | 15.761 | 1.00 | 30.00 | C |
| ATOM | 1209 | C   | ASN | A | 166 | 26.932 | 10.623 | 16.177 | 1.00 | 29.91 | C |
| ATOM | 1210 | O   | ASN | A | 166 | 27.370 | 11.721 | 15.812 | 1.00 | 28.90 | O |
| ATOM | 1211 | CB  | ASN | A | 166 | 24.957 | 11.013 | 14.673 | 1.00 | 29.86 | C |
| ATOM | 1212 | CG  | ASN | A | 166 | 25.720 | 10.957 | 13.363 | 1.00 | 28.91 | C |
| ATOM | 1213 | OD1 | ASN | A | 166 | 26.836 | 10.423 | 13.282 | 1.00 | 27.68 | O |
| ATOM | 1214 | ND2 | ASN | A | 166 | 25.119 | 11.528 | 12.320 | 1.00 | 26.76 | N |
| ATOM | 1215 | N   | TRP | A | 167 | 27.604 | 9.785  | 16.943 | 1.00 | 30.04 | N |
| ATOM | 1216 | CA  | TRP | A | 167 | 28.938 | 10.044 | 17.399 | 1.00 | 30.41 | C |
| ATOM | 1217 | C   | TRP | A | 167 | 29.823 | 10.295 | 16.205 | 1.00 | 30.80 | C |
| ATOM | 1218 | O   | TRP | A | 167 | 30.708 | 11.141 | 16.237 | 1.00 | 30.55 | O |
| ATOM | 1219 | CB  | TRP | A | 167 | 29.390 | 8.847  | 18.232 | 1.00 | 30.31 | C |
| ATOM | 1220 | CG  | TRP | A | 167 | 28.513 | 8.746  | 19.433 | 1.00 | 30.59 | C |
| ATOM | 1221 | CD1 | TRP | A | 167 | 27.594 | 7.792  | 19.699 | 1.00 | 30.51 | C |
| ATOM | 1222 | CD2 | TRP | A | 167 | 28.422 | 9.696  | 20.502 | 1.00 | 31.94 | C |
| ATOM | 1223 | NE1 | TRP | A | 167 | 26.947 | 8.067  | 20.881 | 1.00 | 30.98 | N |
| ATOM | 1224 | CE2 | TRP | A | 167 | 27.442 | 9.232  | 21.395 | 1.00 | 31.41 | C |
| ATOM | 1225 | CE3 | TRP | A | 167 | 29.087 | 10.885 | 20.801 | 1.00 | 31.71 | C |
| ATOM | 1226 | CZ2 | TRP | A | 167 | 27.112 | 9.904  | 22.554 | 1.00 | 32.59 | C |
| ATOM | 1227 | CZ3 | TRP | A | 167 | 28.750 | 11.560 | 21.944 | 1.00 | 32.92 | C |
| ATOM | 1228 | CH2 | TRP | A | 167 | 27.773 | 11.072 | 22.811 | 1.00 | 33.34 | C |
| ATOM | 1229 | N   | ASN | A | 168 | 29.549 | 9.596  | 15.119 | 1.00 | 31.69 | N |
| ATOM | 1230 | CA  | ASN | A | 168 | 30.352 | 9.771  | 13.936 | 1.00 | 32.37 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1231 | C   | ASN | A | 168 | 30.447 | 11.229 | 13.590 | 1.00 | 32.97 | C |
| ATOM | 1232 | O   | ASN | A | 168 | 31.541 | 11.747 | 13.390 | 1.00 | 33.15 | O |
| ATOM | 1233 | CB  | ASN | A | 168 | 29.729 | 9.064  | 12.749 | 1.00 | 32.68 | C |
| ATOM | 1234 | CG  | ASN | A | 168 | 30.594 | 9.147  | 11.507 | 1.00 | 32.86 | C |
| ATOM | 1235 | OD1 | ASN | A | 168 | 31.797 | 8.914  | 11.574 | 1.00 | 35.02 | O |
| ATOM | 1236 | ND2 | ASN | A | 168 | 29.989 | 9.473  | 10.368 | 1.00 | 31.39 | N |
| ATOM | 1237 | N   | TRP | A | 169 | 29.284 | 11.884 | 13.518 | 1.00 | 33.38 | N |
| ATOM | 1238 | CA  | TRP | A | 169 | 29.200 | 13.279 | 13.107 | 1.00 | 33.28 | C |
| ATOM | 1239 | C   | TRP | A | 169 | 29.711 | 14.237 | 14.149 | 1.00 | 33.33 | C |
| ATOM | 1240 | O   | TRP | A | 169 | 30.406 | 15.188 | 13.834 | 1.00 | 33.43 | O |
| ATOM | 1241 | CB  | TRP | A | 169 | 27.756 | 13.673 | 12.765 | 1.00 | 33.43 | C |
| ATOM | 1242 | CG  | TRP | A | 169 | 27.618 | 15.134 | 12.412 | 1.00 | 33.11 | C |
| ATOM | 1243 | CD1 | TRP | A | 169 | 27.814 | 15.698 | 11.191 | 1.00 | 33.49 | C |
| ATOM | 1244 | CD2 | TRP | A | 169 | 27.293 | 16.205 | 13.294 | 1.00 | 32.94 | C |
| ATOM | 1245 | NE1 | TRP | A | 169 | 27.629 | 17.056 | 11.251 | 1.00 | 33.21 | N |
| ATOM | 1246 | CE2 | TRP | A | 169 | 27.306 | 17.397 | 12.533 | 1.00 | 33.42 | C |
| ATOM | 1247 | CE3 | TRP | A | 169 | 26.994 | 16.284 | 14.655 | 1.00 | 33.15 | C |
| ATOM | 1248 | CZ2 | TRP | A | 169 | 27.026 | 18.648 | 13.081 | 1.00 | 33.66 | C |
| ATOM | 1249 | CZ3 | TRP | A | 169 | 26.719 | 17.526 | 15.204 | 1.00 | 34.02 | C |
| ATOM | 1250 | CH2 | TRP | A | 169 | 26.733 | 18.695 | 14.413 | 1.00 | 34.21 | C |
| ATOM | 1251 | N   | ILE | A | 170 | 29.369 | 14.021 | 15.398 | 1.00 | 33.54 | N |
| ATOM | 1252 | CA  | ILE | A | 170 | 29.739 | 15.024 | 16.368 | 1.00 | 33.92 | C |
| ATOM | 1253 | C   | ILE | A | 170 | 31.225 | 14.935 | 16.713 | 1.00 | 34.07 | C |
| ATOM | 1254 | O   | ILE | A | 170 | 31.855 | 15.939 | 16.988 | 1.00 | 34.23 | O |
| ATOM | 1255 | CB  | ILE | A | 170 | 28.832 | 14.947 | 17.591 | 1.00 | 33.84 | C |
| ATOM | 1256 | CG1 | ILE | A | 170 | 28.803 | 16.288 | 18.306 | 1.00 | 34.22 | C |
| ATOM | 1257 | CG2 | ILE | A | 170 | 29.295 | 13.858 | 18.499 | 1.00 | 34.45 | C |
| ATOM | 1258 | CD1 | ILE | A | 170 | 27.869 | 16.309 | 19.478 | 1.00 | 34.73 | C |
| ATOM | 1259 | N   | ASN | A | 171 | 31.801 | 13.743 | 16.650 | 1.00 | 34.41 | N |
| ATOM | 1260 | CA  | ASN | A | 171 | 33.222 | 13.593 | 16.950 | 1.00 | 34.46 | C |
| ATOM | 1261 | C   | ASN | A | 171 | 34.055 | 14.322 | 15.918 | 1.00 | 34.56 | C |
| ATOM | 1262 | O   | ASN | A | 171 | 35.055 | 14.949 | 16.260 | 1.00 | 34.66 | O |
| ATOM | 1263 | CB  | ASN | A | 171 | 33.632 | 12.116 | 16.996 | 1.00 | 34.47 | C |
| ATOM | 1264 | CG  | ASN | A | 171 | 32.969 | 11.356 | 18.128 | 1.00 | 33.99 | C |
| ATOM | 1265 | OD1 | ASN | A | 171 | 32.391 | 11.951 | 19.031 | 1.00 | 35.35 | O |
| ATOM | 1266 | ND2 | ASN | A | 171 | 33.040 | 10.036 | 18.077 | 1.00 | 32.53 | N |
| ATOM | 1267 | N   | LYS | A | 172 | 33.652 | 14.217 | 14.654 | 1.00 | 34.75 | N |
| ATOM | 1268 | CA  | LYS | A | 172 | 34.337 | 14.917 | 13.584 | 1.00 | 35.18 | C |
| ATOM | 1269 | C   | LYS | A | 172 | 34.261 | 16.415 | 13.907 | 1.00 | 35.29 | C |
| ATOM | 1270 | O   | LYS | A | 172 | 35.248 | 17.133 | 13.800 | 1.00 | 34.89 | O |
| ATOM | 1271 | CB  | LYS | A | 172 | 33.711 | 14.600 | 12.216 | 1.00 | 35.26 | C |
| ATOM | 1272 | CG  | LYS | A | 172 | 34.200 | 13.299 | 11.587 | 1.00 | 36.55 | C |
| ATOM | 1273 | CD  | LYS | A | 172 | 33.873 | 13.158 | 10.090 | 1.00 | 38.20 | C |
| ATOM | 1274 | CE  | LYS | A | 172 | 34.512 | 11.872 | 9.537  | 1.00 | 39.82 | C |
| ATOM | 1275 | NZ  | LYS | A | 172 | 34.369 | 11.661 | 8.050  | 1.00 | 41.20 | N |
| ATOM | 1276 | N   | GLN | A | 173 | 33.093 | 16.875 | 14.339 | 1.00 | 35.70 | N |
| ATOM | 1277 | CA  | GLN | A | 173 | 32.931 | 18.272 | 14.699 | 1.00 | 36.20 | C |
| ATOM | 1278 | C   | GLN | A | 173 | 33.929 | 18.633 | 15.771 | 1.00 | 36.47 | C |
| ATOM | 1279 | O   | GLN | A | 173 | 34.605 | 19.656 | 15.686 | 1.00 | 36.97 | O |
| ATOM | 1280 | CB  | GLN | A | 173 | 31.534 | 18.555 | 15.231 | 1.00 | 36.19 | C |
| ATOM | 1281 | CG  | GLN | A | 173 | 30.473 | 18.637 | 14.167 | 1.00 | 36.97 | C |
| ATOM | 1282 | CD  | GLN | A | 173 | 30.765 | 19.720 | 13.157 | 1.00 | 37.19 | C |
| ATOM | 1283 | OE1 | GLN | A | 173 | 31.198 | 20.808 | 13.531 | 1.00 | 38.68 | O |
| ATOM | 1284 | NE2 | GLN | A | 173 | 30.551 | 19.425 | 11.879 | 1.00 | 35.94 | N |
| ATOM | 1285 | N   | GLN | A | 174 | 34.000 | 17.806 | 16.802 | 1.00 | 36.38 | N |
| ATOM | 1286 | CA  | GLN | A | 174 | 34.945 | 18.041 | 17.866 | 1.00 | 36.42 | C |
| ATOM | 1287 | C   | GLN | A | 174 | 36.360 | 18.102 | 17.283 | 1.00 | 36.56 | C |
| ATOM | 1288 | O   | GLN | A | 174 | 37.161 | 18.945 | 17.672 | 1.00 | 36.42 | O |
| ATOM | 1289 | CB  | GLN | A | 174 | 34.815 | 16.937 | 18.912 | 1.00 | 36.33 | C |
| ATOM | 1290 | CG  | GLN | A | 174 | 35.896 | 16.908 | 19.963 | 1.00 | 36.13 | C |
| ATOM | 1291 | CD  | GLN | A | 174 | 35.785 | 15.676 | 20.815 | 1.00 | 36.16 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1292 | OE1 | GLN | A | 174 | 35.415 | 14.613 | 20.314 | 1.00 | 37.84 | O |
| ATOM | 1293 | NE2 | GLN | A | 174 | 36.082 | 15.803 | 22.103 | 1.00 | 34.98 | N |
| ATOM | 1294 | N   | GLY | A | 175 | 36.649 | 17.231 | 16.322 | 1.00 | 36.76 | N |
| ATOM | 1295 | CA  | GLY | A | 175 | 37.976 | 17.158 | 15.750 | 1.00 | 36.97 | C |
| ATOM | 1296 | C   | GLY | A | 175 | 38.302 | 18.356 | 14.892 | 1.00 | 37.21 | C |
| ATOM | 1297 | O   | GLY | A | 175 | 39.336 | 18.993 | 15.070 | 1.00 | 37.38 | O |
| ATOM | 1298 | N   | LYS | A | 176 | 37.406 | 18.682 | 13.971 | 1.00 | 37.44 | N |
| ATOM | 1299 | CA  | LYS | A | 176 | 37.634 | 19.793 | 13.064 | 1.00 | 37.56 | C |
| ATOM | 1300 | C   | LYS | A | 176 | 37.898 | 21.090 | 13.822 | 1.00 | 37.47 | C |
| ATOM | 1301 | O   | LYS | A | 176 | 38.713 | 21.907 | 13.400 | 1.00 | 37.47 | O |
| ATOM | 1302 | CB  | LYS | A | 176 | 36.423 | 20.014 | 12.161 | 1.00 | 37.71 | C |
| ATOM | 1303 | CG  | LYS | A | 176 | 36.134 | 18.905 | 11.163 | 1.00 | 38.70 | C |
| ATOM | 1304 | CD  | LYS | A | 176 | 34.960 | 19.284 | 10.279 | 1.00 | 39.76 | C |
| ATOM | 1305 | CE  | LYS | A | 176 | 34.064 | 18.092 | 10.037 | 1.00 | 41.48 | C |
| ATOM | 1306 | NZ  | LYS | A | 176 | 32.663 | 18.481 | 9.690  | 1.00 | 43.43 | N |
| ATOM | 1307 | N   | ARG | A | 177 | 37.212 | 21.283 | 14.938 | 1.00 | 37.10 | N |
| ATOM | 1308 | CA  | ARG | A | 177 | 37.325 | 22.544 | 15.643 | 1.00 | 37.08 | C |
| ATOM | 1309 | C   | ARG | A | 177 | 38.352 | 22.495 | 16.763 | 1.00 | 36.85 | C |
| ATOM | 1310 | O   | ARG | A | 177 | 38.445 | 23.420 | 17.564 | 1.00 | 36.21 | O |
| ATOM | 1311 | CB  | ARG | A | 177 | 35.980 | 22.969 | 16.228 | 1.00 | 37.21 | C |
| ATOM | 1312 | CG  | ARG | A | 177 | 34.807 | 22.773 | 15.326 | 1.00 | 37.50 | C |
| ATOM | 1313 | CD  | ARG | A | 177 | 34.802 | 23.591 | 14.053 | 1.00 | 38.49 | C |
| ATOM | 1314 | NE  | ARG | A | 177 | 33.750 | 23.066 | 13.185 | 1.00 | 39.56 | N |
| ATOM | 1315 | CZ  | ARG | A | 177 | 33.884 | 22.803 | 11.891 | 1.00 | 41.17 | C |
| ATOM | 1316 | NH1 | ARG | A | 177 | 35.026 | 23.050 | 11.254 | 1.00 | 41.34 | N |
| ATOM | 1317 | NH2 | ARG | A | 177 | 32.855 | 22.304 | 11.219 | 1.00 | 41.89 | N |
| ATOM | 1318 | N   | GLY | A | 178 | 39.088 | 21.401 | 16.859 | 1.00 | 36.70 | N |
| ATOM | 1319 | CA  | GLY | A | 178 | 40.131 | 21.337 | 17.854 | 1.00 | 36.74 | C |
| ATOM | 1320 | C   | GLY | A | 178 | 39.592 | 21.509 | 19.249 | 1.00 | 36.76 | C |
| ATOM | 1321 | O   | GLY | A | 178 | 40.340 | 21.817 | 20.171 | 1.00 | 37.18 | O |
| ATOM | 1322 | N   | TRP | A | 179 | 38.293 | 21.331 | 19.420 | 1.00 | 36.75 | N |
| ATOM | 1323 | CA  | TRP | A | 179 | 37.722 | 21.439 | 20.745 | 1.00 | 36.66 | C |
| ATOM | 1324 | C   | TRP | A | 179 | 38.309 | 20.400 | 21.679 | 1.00 | 36.60 | C |
| ATOM | 1325 | O   | TRP | A | 179 | 38.980 | 19.451 | 21.260 | 1.00 | 35.99 | O |
| ATOM | 1326 | CB  | TRP | A | 179 | 36.222 | 21.216 | 20.708 | 1.00 | 36.79 | C |
| ATOM | 1327 | CG  | TRP | A | 179 | 35.454 | 22.258 | 20.038 | 1.00 | 36.51 | C |
| ATOM | 1328 | CD1 | TRP | A | 179 | 35.889 | 23.470 | 19.620 | 1.00 | 36.67 | C |
| ATOM | 1329 | CD2 | TRP | A | 179 | 34.081 | 22.180 | 19.692 | 1.00 | 37.40 | C |
| ATOM | 1330 | NE1 | TRP | A | 179 | 34.860 | 24.168 | 19.035 | 1.00 | 36.91 | N |
| ATOM | 1331 | CE2 | TRP | A | 179 | 33.735 | 23.390 | 19.062 | 1.00 | 37.43 | C |
| ATOM | 1332 | CE3 | TRP | A | 179 | 33.099 | 21.198 | 19.840 | 1.00 | 36.64 | C |
| ATOM | 1333 | CZ2 | TRP | A | 179 | 32.456 | 23.641 | 18.583 | 1.00 | 36.83 | C |
| ATOM | 1334 | CZ3 | TRP | A | 179 | 31.840 | 21.450 | 19.365 | 1.00 | 36.84 | C |
| ATOM | 1335 | CH2 | TRP | A | 179 | 31.524 | 22.661 | 18.744 | 1.00 | 36.02 | C |
| ATOM | 1336 | N   | GLY | A | 180 | 38.022 | 20.595 | 22.958 | 1.00 | 36.66 | N |
| ATOM | 1337 | CA  | GLY | A | 180 | 38.444 | 19.681 | 23.992 | 1.00 | 36.96 | C |
| ATOM | 1338 | C   | GLY | A | 180 | 37.456 | 18.548 | 24.131 | 1.00 | 37.25 | C |
| ATOM | 1339 | O   | GLY | A | 180 | 36.698 | 18.285 | 23.204 | 1.00 | 37.69 | O |
| ATOM | 1340 | N   | GLN | A | 181 | 37.445 | 17.891 | 25.288 | 1.00 | 37.46 | N |
| ATOM | 1341 | CA  | GLN | A | 181 | 36.581 | 16.734 | 25.507 | 1.00 | 37.81 | C |
| ATOM | 1342 | C   | GLN | A | 181 | 35.136 | 17.088 | 25.802 | 1.00 | 37.40 | C |
| ATOM | 1343 | O   | GLN | A | 181 | 34.825 | 18.177 | 26.273 | 1.00 | 37.59 | O |
| ATOM | 1344 | CB  | GLN | A | 181 | 37.082 | 15.881 | 26.680 | 1.00 | 38.18 | C |
| ATOM | 1345 | CG  | GLN | A | 181 | 36.684 | 16.433 | 28.065 | 1.00 | 40.32 | C |
| ATOM | 1346 | CD  | GLN | A | 181 | 36.956 | 15.470 | 29.231 | 1.00 | 43.44 | C |
| ATOM | 1347 | OE1 | GLN | A | 181 | 38.004 | 14.802 | 29.284 | 1.00 | 44.84 | O |
| ATOM | 1348 | NE2 | GLN | A | 181 | 36.007 | 15.406 | 30.173 | 1.00 | 44.80 | N |
| ATOM | 1349 | N   | LEU | A | 182 | 34.266 | 16.130 | 25.510 | 1.00 | 37.00 | N |
| ATOM | 1350 | CA  | LEU | A | 182 | 32.866 | 16.181 | 25.878 | 1.00 | 36.47 | C |
| ATOM | 1351 | C   | LEU | A | 182 | 32.856 | 16.224 | 27.385 | 1.00 | 35.97 | C |
| ATOM | 1352 | O   | LEU | A | 182 | 33.345 | 15.298 | 28.009 | 1.00 | 35.98 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1353 | CB  | LEU | A | 182 | 32.208 | 14.865 | 25.468 | 1.00 | 36.38 | C |
| ATOM | 1354 | CG  | LEU | A | 182 | 30.691 | 14.707 | 25.336 | 1.00 | 36.76 | C |
| ATOM | 1355 | CD1 | LEU | A | 182 | 30.339 | 13.254 | 25.433 | 1.00 | 36.70 | C |
| ATOM | 1356 | CD2 | LEU | A | 182 | 29.917 | 15.417 | 26.376 | 1.00 | 37.66 | C |
| ATOM | 1357 | N   | THR | A | 183 | 32.337 | 17.270 | 28.005 | 1.00 | 35.50 | N |
| ATOM | 1358 | CA  | THR | A | 183 | 32.310 | 17.230 | 29.457 | 1.00 | 35.07 | C |
| ATOM | 1359 | C   | THR | A | 183 | 31.008 | 16.669 | 29.929 | 1.00 | 34.39 | C |
| ATOM | 1360 | O   | THR | A | 183 | 30.944 | 16.097 | 31.000 | 1.00 | 34.13 | O |
| ATOM | 1361 | CB  | THR | A | 183 | 32.528 | 18.599 | 30.105 | 1.00 | 35.07 | C |
| ATOM | 1362 | OG1 | THR | A | 183 | 31.402 | 19.444 | 29.883 | 1.00 | 35.21 | O |
| ATOM | 1363 | CG2 | THR | A | 183 | 33.652 | 19.310 | 29.453 | 1.00 | 35.76 | C |
| ATOM | 1364 | N   | SER | A | 184 | 29.947 | 16.848 | 29.163 | 1.00 | 33.83 | N |
| ATOM | 1365 | CA  | SER | A | 184 | 28.710 | 16.288 | 29.626 | 1.00 | 33.19 | C |
| ATOM | 1366 | C   | SER | A | 184 | 27.563 | 16.459 | 28.684 | 1.00 | 32.72 | C |
| ATOM | 1367 | O   | SER | A | 184 | 27.643 | 17.172 | 27.699 | 1.00 | 32.59 | O |
| ATOM | 1368 | CB  | SER | A | 184 | 28.363 | 16.954 | 30.949 | 1.00 | 33.18 | C |
| ATOM | 1369 | OG  | SER | A | 184 | 28.349 | 18.347 | 30.788 | 1.00 | 31.82 | O |
| ATOM | 1370 | N   | ASN | A | 185 | 26.484 | 15.776 | 29.013 | 1.00 | 32.44 | N |
| ATOM | 1371 | CA  | ASN | A | 185 | 25.259 | 15.893 | 28.277 | 1.00 | 32.59 | C |
| ATOM | 1372 | C   | ASN | A | 185 | 24.218 | 16.117 | 29.319 | 1.00 | 33.00 | C |
| ATOM | 1373 | O   | ASN | A | 185 | 24.027 | 15.285 | 30.184 | 1.00 | 32.72 | O |
| ATOM | 1374 | CB  | ASN | A | 185 | 24.917 | 14.619 | 27.520 | 1.00 | 32.46 | C |
| ATOM | 1375 | CG  | ASN | A | 185 | 25.850 | 14.351 | 26.369 | 1.00 | 31.69 | C |
| ATOM | 1376 | OD1 | ASN | A | 185 | 26.661 | 13.436 | 26.434 | 1.00 | 32.60 | O |
| ATOM | 1377 | ND2 | ASN | A | 185 | 25.725 | 15.121 | 25.297 | 1.00 | 29.86 | N |
| ATOM | 1378 | N   | LEU | A | 186 | 23.549 | 17.252 | 29.258 | 1.00 | 33.80 | N |
| ATOM | 1379 | CA  | LEU | A | 186 | 22.537 | 17.536 | 30.241 | 1.00 | 34.36 | C |
| ATOM | 1380 | C   | LEU | A | 186 | 21.199 | 17.117 | 29.684 | 1.00 | 34.78 | C |
| ATOM | 1381 | O   | LEU | A | 186 | 20.903 | 17.380 | 28.512 | 1.00 | 35.02 | O |
| ATOM | 1382 | CB  | LEU | A | 186 | 22.500 | 19.029 | 30.539 | 1.00 | 34.34 | C |
| ATOM | 1383 | CG  | LEU | A | 186 | 21.564 | 19.433 | 31.677 | 1.00 | 35.25 | C |
| ATOM | 1384 | CD1 | LEU | A | 186 | 22.122 | 18.827 | 32.930 | 1.00 | 35.58 | C |
| ATOM | 1385 | CD2 | LEU | A | 186 | 21.402 | 20.956 | 31.845 | 1.00 | 35.43 | C |
| ATOM | 1386 | N   | LEU | A | 187 | 20.393 | 16.456 | 30.507 | 1.00 | 34.95 | N |
| ATOM | 1387 | CA  | LEU | A | 187 | 19.022 | 16.189 | 30.120 | 1.00 | 35.27 | C |
| ATOM | 1388 | C   | LEU | A | 187 | 18.117 | 17.260 | 30.735 | 1.00 | 35.48 | C |
| ATOM | 1389 | O   | LEU | A | 187 | 18.105 | 17.449 | 31.951 | 1.00 | 35.40 | O |
| ATOM | 1390 | CB  | LEU | A | 187 | 18.593 | 14.805 | 30.563 | 1.00 | 35.33 | C |
| ATOM | 1391 | CG  | LEU | A | 187 | 17.105 | 14.481 | 30.399 | 1.00 | 36.09 | C |
| ATOM | 1392 | CD1 | LEU | A | 187 | 16.624 | 14.525 | 28.969 | 1.00 | 36.40 | C |
| ATOM | 1393 | CD2 | LEU | A | 187 | 16.850 | 13.114 | 30.940 | 1.00 | 36.96 | C |
| ATOM | 1394 | N   | LEU | A | 188 | 17.380 | 17.977 | 29.889 | 1.00 | 35.70 | N |
| ATOM | 1395 | CA  | LEU | A | 188 | 16.466 | 19.005 | 30.362 | 1.00 | 35.89 | C |
| ATOM | 1396 | C   | LEU | A | 188 | 15.047 | 18.668 | 29.972 | 1.00 | 36.32 | C |
| ATOM | 1397 | O   | LEU | A | 188 | 14.738 | 18.548 | 28.792 | 1.00 | 36.89 | O |
| ATOM | 1398 | CB  | LEU | A | 188 | 16.795 | 20.362 | 29.771 | 1.00 | 35.79 | C |
| ATOM | 1399 | CG  | LEU | A | 188 | 18.210 | 20.889 | 29.937 | 1.00 | 35.66 | C |
| ATOM | 1400 | CD1 | LEU | A | 188 | 18.976 | 20.745 | 28.668 | 1.00 | 36.04 | C |
| ATOM | 1401 | CD2 | LEU | A | 188 | 18.125 | 22.328 | 30.284 | 1.00 | 35.23 | C |
| ATOM | 1402 | N   | ILE | A | 189 | 14.184 | 18.514 | 30.967 | 1.00 | 36.45 | N |
| ATOM | 1403 | CA  | ILE | A | 189 | 12.782 | 18.254 | 30.720 | 1.00 | 36.25 | C |
| ATOM | 1404 | C   | ILE | A | 189 | 12.105 | 19.353 | 31.472 | 1.00 | 35.88 | C |
| ATOM | 1405 | O   | ILE | A | 189 | 12.388 | 19.542 | 32.651 | 1.00 | 35.75 | O |
| ATOM | 1406 | CB  | ILE | A | 189 | 12.368 | 16.916 | 31.274 | 1.00 | 36.47 | C |
| ATOM | 1407 | CG1 | ILE | A | 189 | 13.126 | 15.813 | 30.549 | 1.00 | 36.63 | C |
| ATOM | 1408 | CG2 | ILE | A | 189 | 10.865 | 16.748 | 31.143 | 1.00 | 36.55 | C |
| ATOM | 1409 | CD1 | ILE | A | 189 | 12.884 | 14.440 | 31.129 | 1.00 | 36.11 | C |
| ATOM | 1410 | N   | GLY | A | 190 | 11.221 | 20.071 | 30.789 | 1.00 | 35.53 | N |
| ATOM | 1411 | CA  | GLY | A | 190 | 10.614 | 21.257 | 31.344 | 1.00 | 35.37 | C |
| ATOM | 1412 | C   | GLY | A | 190 | 9.184  | 21.420 | 30.921 | 1.00 | 35.23 | C |
| ATOM | 1413 | O   | GLY | A | 190 | 8.748  | 20.857 | 29.930 | 1.00 | 35.26 | O |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1414 | N   | MET | A | 191 | 8.458  | 22.208 | 31.696 | 1.00 | 35.18 | N |
| ATOM | 1415 | CA  | MET | A | 191 | 7.063  | 22.463 | 31.447 | 1.00 | 35.16 | C |
| ATOM | 1416 | C   | MET | A | 191 | 6.916  | 23.584 | 30.446 | 1.00 | 35.00 | C |
| ATOM | 1417 | O   | MET | A | 191 | 7.795  | 24.426 | 30.316 | 1.00 | 35.17 | O |
| ATOM | 1418 | CB  | MET | A | 191 | 6.379  | 22.849 | 32.750 | 1.00 | 35.13 | C |
| ATOM | 1419 | CG  | MET | A | 191 | 6.277  | 21.691 | 33.710 | 1.00 | 35.63 | C |
| ATOM | 1420 | SD  | MET | A | 191 | 5.756  | 22.150 | 35.360 | 1.00 | 35.65 | S |
| ATOM | 1421 | CE  | MET | A | 191 | 4.222  | 22.827 | 35.017 | 1.00 | 36.16 | C |
| ATOM | 1422 | N   | GLU | A | 192 | 5.804  | 23.573 | 29.727 | 1.00 | 34.83 | N |
| ATOM | 1423 | CA  | GLU | A | 192 | 5.492  | 24.626 | 28.791 | 1.00 | 34.74 | C |
| ATOM | 1424 | C   | GLU | A | 192 | 5.585  | 25.955 | 29.511 | 1.00 | 34.72 | C |
| ATOM | 1425 | O   | GLU | A | 192 | 5.184  | 26.067 | 30.674 | 1.00 | 34.67 | O |
| ATOM | 1426 | CB  | GLU | A | 192 | 4.085  | 24.447 | 28.264 | 1.00 | 34.75 | C |
| ATOM | 1427 | CG  | GLU | A | 192 | 3.029  | 24.525 | 29.348 | 1.00 | 35.09 | C |
| ATOM | 1428 | CD  | GLU | A | 192 | 1.669  | 24.117 | 28.842 | 1.00 | 34.97 | C |
| ATOM | 1429 | OE1 | GLU | A | 192 | 1.609  | 23.503 | 27.756 | 1.00 | 33.58 | O |
| ATOM | 1430 | OE2 | GLU | A | 192 | 0.672  | 24.422 | 29.530 | 1.00 | 35.72 | O |
| ATOM | 1431 | N   | GLY | A | 193 | 6.121  | 26.953 | 28.818 | 1.00 | 34.53 | N |
| ATOM | 1432 | CA  | GLY | A | 193 | 6.265  | 28.279 | 29.378 | 1.00 | 34.63 | C |
| ATOM | 1433 | C   | GLY | A | 193 | 7.528  | 28.542 | 30.180 | 1.00 | 34.49 | C |
| ATOM | 1434 | O   | GLY | A | 193 | 7.864  | 29.694 | 30.434 | 1.00 | 34.57 | O |
| ATOM | 1435 | N   | ASN | A | 194 | 8.224  | 27.493 | 30.594 | 1.00 | 34.27 | N |
| ATOM | 1436 | CA  | ASN | A | 194 | 9.441  | 27.672 | 31.367 | 1.00 | 34.06 | C |
| ATOM | 1437 | C   | ASN | A | 194 | 10.466 | 28.492 | 30.609 | 1.00 | 33.93 | C |
| ATOM | 1438 | O   | ASN | A | 194 | 10.552 | 28.415 | 29.392 | 1.00 | 33.84 | O |
| ATOM | 1439 | CB  | ASN | A | 194 | 10.051 | 26.316 | 31.721 | 1.00 | 33.99 | C |
| ATOM | 1440 | CG  | ASN | A | 194 | 9.314  | 25.625 | 32.836 | 1.00 | 33.19 | C |
| ATOM | 1441 | OD1 | ASN | A | 194 | 8.257  | 26.081 | 33.265 | 1.00 | 33.07 | O |
| ATOM | 1442 | ND2 | ASN | A | 194 | 9.869  | 24.528 | 33.323 | 1.00 | 31.93 | N |
| ATOM | 1443 | N   | VAL | A | 195 | 11.243 | 29.285 | 31.332 | 1.00 | 33.86 | N |
| ATOM | 1444 | CA  | VAL | A | 195 | 12.288 | 30.069 | 30.707 | 1.00 | 33.70 | C |
| ATOM | 1445 | C   | VAL | A | 195 | 13.621 | 29.969 | 31.396 | 1.00 | 33.38 | C |
| ATOM | 1446 | O   | VAL | A | 195 | 13.721 | 30.115 | 32.601 | 1.00 | 33.75 | O |
| ATOM | 1447 | CB  | VAL | A | 195 | 11.964 | 31.552 | 30.779 | 1.00 | 33.96 | C |
| ATOM | 1448 | CG1 | VAL | A | 195 | 13.151 | 32.389 | 30.253 | 1.00 | 34.32 | C |
| ATOM | 1449 | CG2 | VAL | A | 195 | 10.693 | 31.854 | 30.032 | 1.00 | 34.15 | C |
| ATOM | 1450 | N   | THR | A | 196 | 14.666 | 29.764 | 30.621 | 1.00 | 33.04 | N |
| ATOM | 1451 | CA  | THR | A | 196 | 15.991 | 29.883 | 31.161 | 1.00 | 32.60 | C |
| ATOM | 1452 | C   | THR | A | 196 | 16.438 | 31.256 | 30.723 | 1.00 | 32.21 | C |
| ATOM | 1453 | O   | THR | A | 196 | 16.584 | 31.500 | 29.530 | 1.00 | 31.64 | O |
| ATOM | 1454 | CB  | THR | A | 196 | 16.887 | 28.836 | 30.586 | 1.00 | 32.68 | C |
| ATOM | 1455 | OG1 | THR | A | 196 | 16.466 | 27.543 | 31.048 | 1.00 | 33.09 | O |
| ATOM | 1456 | CG2 | THR | A | 196 | 18.281 | 29.003 | 31.124 | 1.00 | 32.63 | C |
| ATOM | 1457 | N   | PRO | A | 197 | 16.585 | 32.177 | 31.672 | 1.00 | 31.97 | N |
| ATOM | 1458 | CA  | PRO | A | 197 | 17.000 | 33.530 | 31.350 | 1.00 | 31.74 | C |
| ATOM | 1459 | C   | PRO | A | 197 | 18.385 | 33.564 | 30.816 | 1.00 | 31.92 | C |
| ATOM | 1460 | O   | PRO | A | 197 | 19.215 | 32.717 | 31.129 | 1.00 | 32.52 | O |
| ATOM | 1461 | CB  | PRO | A | 197 | 16.950 | 34.234 | 32.682 | 1.00 | 31.38 | C |
| ATOM | 1462 | CG  | PRO | A | 197 | 16.056 | 33.508 | 33.418 | 1.00 | 31.84 | C |
| ATOM | 1463 | CD  | PRO | A | 197 | 16.305 | 32.055 | 33.107 | 1.00 | 32.08 | C |
| ATOM | 1464 | N   | ALA | A | 198 | 18.615 | 34.592 | 30.024 | 1.00 | 32.06 | N |
| ATOM | 1465 | CA  | ALA | A | 198 | 19.846 | 34.787 | 29.311 | 1.00 | 32.28 | C |
| ATOM | 1466 | C   | ALA | A | 198 | 21.101 | 34.690 | 30.162 | 1.00 | 32.42 | C |
| ATOM | 1467 | O   | ALA | A | 198 | 21.213 | 35.305 | 31.220 | 1.00 | 32.03 | O |
| ATOM | 1468 | CB  | ALA | A | 198 | 19.798 | 36.131 | 28.625 | 1.00 | 32.42 | C |
| ATOM | 1469 | N   | HIS | A | 199 | 22.064 | 33.953 | 29.630 | 1.00 | 32.77 | N |
| ATOM | 1470 | CA  | HIS | A | 199 | 23.339 | 33.737 | 30.271 | 1.00 | 33.31 | C |
| ATOM | 1471 | C   | HIS | A | 199 | 24.308 | 33.252 | 29.220 | 1.00 | 33.76 | C |
| ATOM | 1472 | O   | HIS | A | 199 | 23.902 | 33.013 | 28.084 | 1.00 | 34.10 | O |
| ATOM | 1473 | CB  | HIS | A | 199 | 23.194 | 32.622 | 31.275 | 1.00 | 33.24 | C |
| ATOM | 1474 | CG  | HIS | A | 199 | 22.879 | 31.311 | 30.639 | 1.00 | 32.59 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1475 | ND1 | HIS | A | 199 | 21.602 | 30.958 | 30.269 | 1.00 | 31.40 | N |
| ATOM | 1476 | CD2 | HIS | A | 199 | 23.679 | 30.292 | 30.253 | 1.00 | 32.85 | C |
| ATOM | 1477 | CE1 | HIS | A | 199 | 21.624 | 29.761 | 29.714 | 1.00 | 32.37 | C |
| ATOM | 1478 | NE2 | HIS | A | 199 | 22.871 | 29.330 | 29.698 | 1.00 | 32.78 | N |
| ATOM | 1479 | N   | TYR | A | 200 | 25.575 | 33.093 | 29.601 | 1.00 | 34.35 | N |
| ATOM | 1480 | CA  | TYR | A | 200 | 26.580 | 32.502 | 28.712 | 1.00 | 34.92 | C |
| ATOM | 1481 | C   | TYR | A | 200 | 27.256 | 31.350 | 29.431 | 1.00 | 35.15 | C |
| ATOM | 1482 | O   | TYR | A | 200 | 27.285 | 31.318 | 30.661 | 1.00 | 35.76 | O |
| ATOM | 1483 | CB  | TYR | A | 200 | 27.599 | 33.510 | 28.175 | 1.00 | 34.90 | C |
| ATOM | 1484 | CG  | TYR | A | 200 | 28.586 | 34.096 | 29.156 | 1.00 | 34.89 | C |
| ATOM | 1485 | CD1 | TYR | A | 200 | 29.825 | 33.519 | 29.359 | 1.00 | 33.02 | C |
| ATOM | 1486 | CD2 | TYR | A | 200 | 28.307 | 35.292 | 29.802 | 1.00 | 36.04 | C |
| ATOM | 1487 | CE1 | TYR | A | 200 | 30.731 | 34.079 | 30.224 | 1.00 | 33.25 | C |
| ATOM | 1488 | CE2 | TYR | A | 200 | 29.200 | 35.857 | 30.664 | 1.00 | 35.45 | C |
| ATOM | 1489 | CZ  | TYR | A | 200 | 30.410 | 35.253 | 30.882 | 1.00 | 34.40 | C |
| ATOM | 1490 | OH  | TYR | A | 200 | 31.301 | 35.855 | 31.739 | 1.00 | 32.62 | O |
| ATOM | 1491 | N   | ASP | A | 201 | 27.747 | 30.387 | 28.654 | 1.00 | 35.04 | N |
| ATOM | 1492 | CA  | ASP | A | 201 | 28.386 | 29.189 | 29.182 | 1.00 | 34.82 | C |
| ATOM | 1493 | C   | ASP | A | 201 | 29.818 | 29.220 | 28.652 | 1.00 | 34.87 | C |
| ATOM | 1494 | O   | ASP | A | 201 | 30.047 | 29.734 | 27.588 | 1.00 | 34.81 | O |
| ATOM | 1495 | CB  | ASP | A | 201 | 27.636 | 27.925 | 28.727 | 1.00 | 34.49 | C |
| ATOM | 1496 | CG  | ASP | A | 201 | 26.212 | 27.854 | 29.256 | 1.00 | 34.63 | C |
| ATOM | 1497 | OD1 | ASP | A | 201 | 26.046 | 27.953 | 30.480 | 1.00 | 33.52 | O |
| ATOM | 1498 | OD2 | ASP | A | 201 | 25.191 | 27.680 | 28.533 | 1.00 | 36.84 | O |
| ATOM | 1499 | N   | GLU | A | 202 | 30.795 | 28.727 | 29.399 | 1.00 | 35.74 | N |
| ATOM | 1500 | CA  | GLU | A | 202 | 32.176 | 28.699 | 28.899 | 1.00 | 36.38 | C |
| ATOM | 1501 | C   | GLU | A | 202 | 32.528 | 27.441 | 28.126 | 1.00 | 36.30 | C |
| ATOM | 1502 | O   | GLU | A | 202 | 33.679 | 27.019 | 28.126 | 1.00 | 37.04 | O |
| ATOM | 1503 | CB  | GLU | A | 202 | 33.172 | 28.830 | 30.048 | 1.00 | 36.61 | C |
| ATOM | 1504 | CG  | GLU | A | 202 | 33.100 | 30.185 | 30.725 | 1.00 | 37.81 | C |
| ATOM | 1505 | CD  | GLU | A | 202 | 33.960 | 30.276 | 31.949 | 1.00 | 38.93 | C |
| ATOM | 1506 | OE1 | GLU | A | 202 | 33.525 | 29.783 | 33.020 | 1.00 | 39.85 | O |
| ATOM | 1507 | OE2 | GLU | A | 202 | 35.055 | 30.858 | 31.832 | 1.00 | 40.19 | O |
| ATOM | 1508 | N   | GLN | A | 203 | 31.556 | 26.840 | 27.462 | 1.00 | 35.68 | N |
| ATOM | 1509 | CA  | GLN | A | 203 | 31.815 | 25.643 | 26.718 | 1.00 | 35.24 | C |
| ATOM | 1510 | C   | GLN | A | 203 | 31.107 | 25.754 | 25.406 | 1.00 | 34.57 | C |
| ATOM | 1511 | O   | GLN | A | 203 | 30.218 | 26.586 | 25.256 | 1.00 | 34.62 | O |
| ATOM | 1512 | CB  | GLN | A | 203 | 31.317 | 24.446 | 27.514 | 1.00 | 35.59 | C |
| ATOM | 1513 | CG  | GLN | A | 203 | 32.184 | 24.236 | 28.734 | 1.00 | 37.42 | C |
| ATOM | 1514 | CD  | GLN | A | 203 | 32.234 | 22.819 | 29.233 | 1.00 | 38.70 | C |
| ATOM | 1515 | OE1 | GLN | A | 203 | 32.228 | 21.860 | 28.458 | 1.00 | 39.80 | O |
| ATOM | 1516 | NE2 | GLN | A | 203 | 32.326 | 22.680 | 30.541 | 1.00 | 41.01 | N |
| ATOM | 1517 | N   | GLN | A | 204 | 31.524 | 24.939 | 24.443 | 1.00 | 33.68 | N |
| ATOM | 1518 | CA  | GLN | A | 204 | 30.873 | 24.899 | 23.165 | 1.00 | 32.97 | C |
| ATOM | 1519 | C   | GLN | A | 204 | 29.714 | 23.959 | 23.373 | 1.00 | 32.67 | C |
| ATOM | 1520 | O   | GLN | A | 204 | 29.838 | 22.982 | 24.082 | 1.00 | 32.33 | O |
| ATOM | 1521 | CB  | GLN | A | 204 | 31.793 | 24.352 | 22.093 | 1.00 | 32.85 | C |
| ATOM | 1522 | CG  | GLN | A | 204 | 33.042 | 25.165 | 21.819 | 1.00 | 32.50 | C |
| ATOM | 1523 | CD  | GLN | A | 204 | 32.786 | 26.454 | 21.057 | 1.00 | 30.59 | C |
| ATOM | 1524 | OE1 | GLN | A | 204 | 31.656 | 26.830 | 20.848 | 1.00 | 31.27 | O |
| ATOM | 1525 | NE2 | GLN | A | 204 | 33.843 | 27.132 | 20.664 | 1.00 | 29.18 | N |
| ATOM | 1526 | N   | ASN | A | 205 | 28.583 | 24.247 | 22.755 | 1.00 | 32.81 | N |
| ATOM | 1527 | CA  | ASN | A | 205 | 27.393 | 23.446 | 22.980 | 1.00 | 32.85 | C |
| ATOM | 1528 | C   | ASN | A | 205 | 26.594 | 23.059 | 21.733 | 1.00 | 32.80 | C |
| ATOM | 1529 | O   | ASN | A | 205 | 26.147 | 23.921 | 20.968 | 1.00 | 32.72 | O |
| ATOM | 1530 | CB  | ASN | A | 205 | 26.484 | 24.246 | 23.919 | 1.00 | 32.83 | C |
| ATOM | 1531 | CG  | ASN | A | 205 | 25.178 | 23.566 | 24.205 | 1.00 | 32.43 | C |
| ATOM | 1532 | OD1 | ASN | A | 205 | 24.914 | 22.465 | 23.732 | 1.00 | 32.78 | O |
| ATOM | 1533 | ND2 | ASN | A | 205 | 24.339 | 24.228 | 24.993 | 1.00 | 31.52 | N |
| ATOM | 1534 | N   | PHE | A | 206 | 26.427 | 21.763 | 21.515 | 1.00 | 32.36 | N |
| ATOM | 1535 | CA  | PHE | A | 206 | 25.454 | 21.326 | 20.541 | 1.00 | 32.02 | C |



|      |      |     |           |        |        |        |      |       |   |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 1536 | C   | PHE A 206 | 24.167 | 20.977 | 21.301 | 1.00 | 31.59 | C |
| ATOM | 1537 | O   | PHE A 206 | 24.144 | 20.067 | 22.096 | 1.00 | 31.13 | O |
| ATOM | 1538 | CB  | PHE A 206 | 25.972 | 20.159 | 19.754 | 1.00 | 32.17 | C |
| ATOM | 1539 | CG  | PHE A 206 | 26.844 | 20.554 | 18.639 | 1.00 | 32.42 | C |
| ATOM | 1540 | CD1 | PHE A 206 | 26.364 | 21.354 | 17.630 | 1.00 | 33.16 | C |
| ATOM | 1541 | CD2 | PHE A 206 | 28.149 | 20.132 | 18.600 | 1.00 | 33.19 | C |
| ATOM | 1542 | CE1 | PHE A 206 | 27.174 | 21.721 | 16.600 | 1.00 | 33.34 | C |
| ATOM | 1543 | CE2 | PHE A 206 | 28.963 | 20.487 | 17.580 | 1.00 | 32.88 | C |
| ATOM | 1544 | CZ  | PHE A 206 | 28.485 | 21.279 | 16.574 | 1.00 | 33.50 | C |
| ATOM | 1545 | N   | PHE A 207 | 23.104 | 21.717 | 21.012 | 1.00 | 31.65 | N |
| ATOM | 1546 | CA  | PHE A 207 | 21.829 | 21.671 | 21.726 | 1.00 | 31.71 | C |
| ATOM | 1547 | C   | PHE A 207 | 20.822 | 20.825 | 20.924 | 1.00 | 31.35 | C |
| ATOM | 1548 | O   | PHE A 207 | 20.289 | 21.292 | 19.930 | 1.00 | 30.81 | O |
| ATOM | 1549 | CB  | PHE A 207 | 21.391 | 23.148 | 21.883 | 1.00 | 31.56 | C |
| ATOM | 1550 | CG  | PHE A 207 | 20.118 | 23.404 | 22.683 | 1.00 | 31.43 | C |
| ATOM | 1551 | CD1 | PHE A 207 | 18.926 | 23.676 | 22.036 | 1.00 | 32.30 | C |
| ATOM | 1552 | CD2 | PHE A 207 | 20.150 | 23.519 | 24.058 | 1.00 | 31.29 | C |
| ATOM | 1553 | CE1 | PHE A 207 | 17.781 | 23.982 | 22.748 | 1.00 | 32.37 | C |
| ATOM | 1554 | CE2 | PHE A 207 | 19.006 | 23.832 | 24.776 | 1.00 | 31.14 | C |
| ATOM | 1555 | CZ  | PHE A 207 | 17.828 | 24.062 | 24.122 | 1.00 | 32.27 | C |
| ATOM | 1556 | N   | ALA A 208 | 20.554 | 19.593 | 21.368 | 1.00 | 31.31 | N |
| ATOM | 1557 | CA  | ALA A 208 | 19.685 | 18.672 | 20.611 | 1.00 | 31.33 | C |
| ATOM | 1558 | C   | ALA A 208 | 18.264 | 18.543 | 21.138 | 1.00 | 31.59 | C |
| ATOM | 1559 | O   | ALA A 208 | 18.016 | 17.860 | 22.133 | 1.00 | 31.13 | O |
| ATOM | 1560 | CB  | ALA A 208 | 20.293 | 17.334 | 20.537 | 1.00 | 30.98 | C |
| ATOM | 1561 | N   | GLN A 209 | 17.340 | 19.169 | 20.409 | 1.00 | 32.00 | N |
| ATOM | 1562 | CA  | GLN A 209 | 15.935 | 19.183 | 20.751 | 1.00 | 32.37 | C |
| ATOM | 1563 | C   | GLN A 209 | 15.288 | 17.867 | 20.358 | 1.00 | 32.76 | C |
| ATOM | 1564 | O   | GLN A 209 | 15.492 | 17.360 | 19.247 | 1.00 | 32.19 | O |
| ATOM | 1565 | CB  | GLN A 209 | 15.245 | 20.332 | 20.031 | 1.00 | 32.55 | C |
| ATOM | 1566 | CG  | GLN A 209 | 13.802 | 20.589 | 20.470 | 1.00 | 32.44 | C |
| ATOM | 1567 | CD  | GLN A 209 | 13.689 | 20.978 | 21.925 | 1.00 | 32.27 | C |
| ATOM | 1568 | OE1 | GLN A 209 | 14.699 | 21.254 | 22.587 | 1.00 | 31.73 | O |
| ATOM | 1569 | NE2 | GLN A 209 | 12.457 | 21.000 | 22.436 | 1.00 | 32.63 | N |
| ATOM | 1570 | N   | ILE A 210 | 14.467 | 17.360 | 21.272 | 1.00 | 33.20 | N |
| ATOM | 1571 | CA  | ILE A 210 | 13.907 | 16.030 | 21.165 | 1.00 | 33.55 | C |
| ATOM | 1572 | C   | ILE A 210 | 12.399 | 15.998 | 21.195 | 1.00 | 33.37 | C |
| ATOM | 1573 | O   | ILE A 210 | 11.788 | 15.337 | 20.369 | 1.00 | 33.25 | O |
| ATOM | 1574 | CB  | ILE A 210 | 14.456 | 15.210 | 22.302 | 1.00 | 33.79 | C |
| ATOM | 1575 | CG1 | ILE A 210 | 15.900 | 14.837 | 21.980 | 1.00 | 34.71 | C |
| ATOM | 1576 | CG2 | ILE A 210 | 13.604 | 13.982 | 22.528 | 1.00 | 33.99 | C |
| ATOM | 1577 | CD1 | ILE A 210 | 16.679 | 14.375 | 23.191 | 1.00 | 35.48 | C |
| ATOM | 1578 | N   | LYS A 211 | 11.804 | 16.688 | 22.156 | 1.00 | 33.27 | N |
| ATOM | 1579 | CA  | LYS A 211 | 10.365 | 16.739 | 22.263 | 1.00 | 33.48 | C |
| ATOM | 1580 | C   | LYS A 211 | 9.960  | 18.146 | 22.559 | 1.00 | 33.68 | C |
| ATOM | 1581 | O   | LYS A 211 | 10.545 | 18.789 | 23.407 | 1.00 | 34.10 | O |
| ATOM | 1582 | CB  | LYS A 211 | 9.867  | 15.875 | 23.405 | 1.00 | 33.57 | C |
| ATOM | 1583 | CG  | LYS A 211 | 8.355  | 15.708 | 23.409 | 1.00 | 34.06 | C |
| ATOM | 1584 | CD  | LYS A 211 | 7.840  | 15.250 | 24.752 | 1.00 | 34.79 | C |
| ATOM | 1585 | CE  | LYS A 211 | 6.635  | 14.324 | 24.635 | 1.00 | 35.65 | C |
| ATOM | 1586 | NZ  | LYS A 211 | 5.876  | 14.398 | 23.369 | 1.00 | 36.67 | N |
| ATOM | 1587 | N   | GLY A 212 | 8.938  | 18.626 | 21.876 | 1.00 | 34.06 | N |
| ATOM | 1588 | CA  | GLY A 212 | 8.460  | 19.969 | 22.103 | 1.00 | 34.09 | C |
| ATOM | 1589 | C   | GLY A 212 | 9.270  | 20.966 | 21.314 | 1.00 | 34.27 | C |
| ATOM | 1590 | O   | GLY A 212 | 10.156 | 20.599 | 20.532 | 1.00 | 34.27 | O |
| ATOM | 1591 | N   | TYR A 213 | 8.955  | 22.237 | 21.523 | 1.00 | 34.23 | N |
| ATOM | 1592 | CA  | TYR A 213 | 9.640  | 23.311 | 20.843 | 1.00 | 34.12 | C |
| ATOM | 1593 | C   | TYR A 213 | 10.216 | 24.318 | 21.824 | 1.00 | 33.81 | C |
| ATOM | 1594 | O   | TYR A 213 | 9.602  | 24.652 | 22.835 | 1.00 | 33.09 | O |
| ATOM | 1595 | CB  | TYR A 213 | 8.665  | 23.994 | 19.899 | 1.00 | 34.42 | C |
| ATOM | 1596 | CG  | TYR A 213 | 8.257  | 23.091 | 18.789 | 1.00 | 35.40 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1597 | CD1 | TYR | A | 213 | 7.228  | 22.163 | 18.955 | 1.00 | 36.80 | C |
| ATOM | 1598 | CD2 | TYR | A | 213 | 8.929  | 23.122 | 17.586 | 1.00 | 36.00 | C |
| ATOM | 1599 | CE1 | TYR | A | 213 | 6.873  | 21.323 | 17.944 | 1.00 | 36.82 | C |
| ATOM | 1600 | CE2 | TYR | A | 213 | 8.579  | 22.292 | 16.567 | 1.00 | 37.06 | C |
| ATOM | 1601 | CZ  | TYR | A | 213 | 7.560  | 21.390 | 16.743 | 1.00 | 37.82 | C |
| ATOM | 1602 | OH  | TYR | A | 213 | 7.242  | 20.568 | 15.688 | 1.00 | 40.76 | O |
| ATOM | 1603 | N   | LYS | A | 214 | 11.410 | 24.804 | 21.517 | 1.00 | 33.91 | N |
| ATOM | 1604 | CA  | LYS | A | 214 | 12.046 | 25.809 | 22.359 | 1.00 | 33.87 | C |
| ATOM | 1605 | C   | LYS | A | 214 | 12.479 | 27.033 | 21.551 | 1.00 | 33.71 | C |
| ATOM | 1606 | O   | LYS | A | 214 | 13.173 | 26.918 | 20.538 | 1.00 | 33.58 | O |
| ATOM | 1607 | CB  | LYS | A | 214 | 13.237 | 25.208 | 23.101 | 1.00 | 33.64 | C |
| ATOM | 1608 | CG  | LYS | A | 214 | 12.881 | 24.443 | 24.364 | 1.00 | 33.56 | C |
| ATOM | 1609 | CD  | LYS | A | 214 | 14.126 | 23.861 | 24.973 | 1.00 | 33.29 | C |
| ATOM | 1610 | CE  | LYS | A | 214 | 14.001 | 23.615 | 26.458 | 1.00 | 33.54 | C |
| ATOM | 1611 | NZ  | LYS | A | 214 | 15.346 | 23.419 | 27.130 | 1.00 | 32.27 | N |
| ATOM | 1612 | N   | ARG | A | 215 | 12.043 | 28.205 | 21.986 | 1.00 | 33.56 | N |
| ATOM | 1613 | CA  | ARG | A | 215 | 12.479 | 29.427 | 21.339 | 1.00 | 33.91 | C |
| ATOM | 1614 | C   | ARG | A | 215 | 13.816 | 29.800 | 21.944 | 1.00 | 33.54 | C |
| ATOM | 1615 | O   | ARG | A | 215 | 13.946 | 29.923 | 23.146 | 1.00 | 32.78 | O |
| ATOM | 1616 | CB  | ARG | A | 215 | 11.482 | 30.552 | 21.558 | 1.00 | 34.15 | C |
| ATOM | 1617 | CG  | ARG | A | 215 | 11.865 | 31.844 | 20.885 | 1.00 | 34.51 | C |
| ATOM | 1618 | CD  | ARG | A | 215 | 11.287 | 33.028 | 21.593 | 1.00 | 34.99 | C |
| ATOM | 1619 | NE  | ARG | A | 215 | 11.381 | 34.255 | 20.823 | 1.00 | 35.43 | N |
| ATOM | 1620 | CZ  | ARG | A | 215 | 10.688 | 35.346 | 21.103 | 1.00 | 35.27 | C |
| ATOM | 1621 | NH1 | ARG | A | 215 | 9.860  | 35.371 | 22.144 | 1.00 | 34.68 | N |
| ATOM | 1622 | NH2 | ARG | A | 215 | 10.829 | 36.415 | 20.344 | 1.00 | 35.16 | N |
| ATOM | 1623 | N   | CYS | A | 216 | 14.810 | 29.962 | 21.092 | 1.00 | 33.76 | N |
| ATOM | 1624 | CA  | CYS | A | 216 | 16.152 | 30.238 | 21.542 | 1.00 | 33.91 | C |
| ATOM | 1625 | C   | CYS | A | 216 | 16.555 | 31.613 | 21.068 | 1.00 | 34.31 | C |
| ATOM | 1626 | O   | CYS | A | 216 | 16.534 | 31.885 | 19.872 | 1.00 | 34.69 | O |
| ATOM | 1627 | CB  | CYS | A | 216 | 17.099 | 29.189 | 20.968 | 1.00 | 33.84 | C |
| ATOM | 1628 | SG  | CYS | A | 216 | 16.655 | 27.490 | 21.397 | 1.00 | 32.85 | S |
| ATOM | 1629 | N   | ILE | A | 217 | 16.886 | 32.494 | 22.004 | 1.00 | 34.57 | N |
| ATOM | 1630 | CA  | ILE | A | 217 | 17.335 | 33.830 | 21.648 | 1.00 | 34.82 | C |
| ATOM | 1631 | C   | ILE | A | 217 | 18.785 | 33.999 | 22.046 | 1.00 | 34.50 | C |
| ATOM | 1632 | O   | ILE | A | 217 | 19.136 | 33.839 | 23.213 | 1.00 | 34.30 | O |
| ATOM | 1633 | CB  | ILE | A | 217 | 16.475 | 34.890 | 22.324 | 1.00 | 35.07 | C |
| ATOM | 1634 | CG1 | ILE | A | 217 | 15.003 | 34.652 | 22.001 | 1.00 | 35.20 | C |
| ATOM | 1635 | CG2 | ILE | A | 217 | 16.881 | 36.259 | 21.844 | 1.00 | 35.38 | C |
| ATOM | 1636 | CD1 | ILE | A | 217 | 14.086 | 35.585 | 22.722 | 1.00 | 36.16 | C |
| ATOM | 1637 | N   | LEU | A | 218 | 19.620 | 34.315 | 21.060 | 1.00 | 34.32 | N |
| ATOM | 1638 | CA  | LEU | A | 218 | 21.052 | 34.443 | 21.277 | 1.00 | 34.44 | C |
| ATOM | 1639 | C   | LEU | A | 218 | 21.565 | 35.844 | 21.017 | 1.00 | 34.27 | C |
| ATOM | 1640 | O   | LEU | A | 218 | 21.074 | 36.561 | 20.148 | 1.00 | 34.59 | O |
| ATOM | 1641 | CB  | LEU | A | 218 | 21.818 | 33.476 | 20.365 | 1.00 | 34.57 | C |
| ATOM | 1642 | CG  | LEU | A | 218 | 21.953 | 32.036 | 20.844 | 1.00 | 34.62 | C |
| ATOM | 1643 | CD1 | LEU | A | 218 | 20.614 | 31.435 | 21.124 | 1.00 | 34.96 | C |
| ATOM | 1644 | CD2 | LEU | A | 218 | 22.638 | 31.235 | 19.789 | 1.00 | 35.31 | C |
| ATOM | 1645 | N   | PHE | A | 219 | 22.594 | 36.200 | 21.768 | 1.00 | 33.79 | N |
| ATOM | 1646 | CA  | PHE | A | 219 | 23.258 | 37.462 | 21.632 | 1.00 | 33.40 | C |
| ATOM | 1647 | C   | PHE | A | 219 | 24.730 | 37.155 | 21.617 | 1.00 | 33.29 | C |
| ATOM | 1648 | O   | PHE | A | 219 | 25.222 | 36.434 | 22.463 | 1.00 | 33.45 | O |
| ATOM | 1649 | CB  | PHE | A | 219 | 22.964 | 38.330 | 22.832 | 1.00 | 33.37 | C |
| ATOM | 1650 | CG  | PHE | A | 219 | 21.509 | 38.586 | 23.051 | 1.00 | 33.91 | C |
| ATOM | 1651 | CD1 | PHE | A | 219 | 20.852 | 39.607 | 22.379 | 1.00 | 33.73 | C |
| ATOM | 1652 | CD2 | PHE | A | 219 | 20.794 | 37.812 | 23.942 | 1.00 | 33.70 | C |
| ATOM | 1653 | CE1 | PHE | A | 219 | 19.512 | 39.832 | 22.600 | 1.00 | 33.52 | C |
| ATOM | 1654 | CE2 | PHE | A | 219 | 19.460 | 38.038 | 24.156 | 1.00 | 33.47 | C |
| ATOM | 1655 | CZ  | PHE | A | 219 | 18.818 | 39.045 | 23.486 | 1.00 | 33.23 | C |
| ATOM | 1656 | N   | PRO | A | 220 | 25.438 | 37.683 | 20.642 | 1.00 | 33.46 | N |
| ATOM | 1657 | CA  | PRO | A | 220 | 26.888 | 37.496 | 20.536 | 1.00 | 33.50 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1658 | C   | PRO | A | 220 | 27.675 | 38.131 | 21.699 | 1.00 | 33.51 | C |
| ATOM | 1659 | O   | PRO | A | 220 | 27.185 | 39.049 | 22.363 | 1.00 | 33.18 | O |
| ATOM | 1660 | CB  | PRO | A | 220 | 27.246 | 38.169 | 19.211 | 1.00 | 33.51 | C |
| ATOM | 1661 | CG  | PRO | A | 220 | 25.977 | 38.683 | 18.629 | 1.00 | 33.41 | C |
| ATOM | 1662 | CD  | PRO | A | 220 | 24.869 | 38.462 | 19.544 | 1.00 | 33.33 | C |
| ATOM | 1663 | N   | PRO | A | 221 | 28.886 | 37.627 | 21.942 | 1.00 | 33.38 | N |
| ATOM | 1664 | CA  | PRO | A | 221 | 29.731 | 38.102 | 23.044 | 1.00 | 33.30 | C |
| ATOM | 1665 | C   | PRO | A | 221 | 29.966 | 39.581 | 23.081 | 1.00 | 33.55 | C |
| ATOM | 1666 | O   | PRO | A | 221 | 30.043 | 40.151 | 24.147 | 1.00 | 33.66 | O |
| ATOM | 1667 | CB  | PRO | A | 221 | 31.033 | 37.375 | 22.799 | 1.00 | 33.11 | C |
| ATOM | 1668 | CG  | PRO | A | 221 | 30.589 | 36.128 | 22.147 | 1.00 | 33.06 | C |
| ATOM | 1669 | CD  | PRO | A | 221 | 29.523 | 36.522 | 21.207 | 1.00 | 32.91 | C |
| ATOM | 1670 | N   | ASP | A | 222 | 30.009 | 40.217 | 21.933 | 1.00 | 34.30 | N |
| ATOM | 1671 | CA  | ASP | A | 222 | 30.277 | 41.628 | 21.904 | 1.00 | 34.71 | C |
| ATOM | 1672 | C   | ASP | A | 222 | 29.073 | 42.419 | 22.382 | 1.00 | 34.56 | C |
| ATOM | 1673 | O   | ASP | A | 222 | 29.048 | 43.634 | 22.241 | 1.00 | 34.68 | O |
| ATOM | 1674 | CB  | ASP | A | 222 | 30.679 | 42.055 | 20.502 | 1.00 | 34.79 | C |
| ATOM | 1675 | CG  | ASP | A | 222 | 29.508 | 42.228 | 19.608 | 1.00 | 36.26 | C |
| ATOM | 1676 | OD1 | ASP | A | 222 | 28.387 | 41.897 | 20.028 | 1.00 | 38.21 | O |
| ATOM | 1677 | OD2 | ASP | A | 222 | 29.601 | 42.692 | 18.462 | 1.00 | 40.87 | O |
| ATOM | 1678 | N   | GLN | A | 223 | 28.062 | 41.760 | 22.930 | 1.00 | 34.48 | N |
| ATOM | 1679 | CA  | GLN | A | 223 | 26.965 | 42.532 | 23.497 | 1.00 | 34.78 | C |
| ATOM | 1680 | C   | GLN | A | 223 | 27.031 | 42.541 | 25.011 | 1.00 | 34.33 | C |
| ATOM | 1681 | O   | GLN | A | 223 | 26.077 | 42.878 | 25.686 | 1.00 | 34.70 | O |
| ATOM | 1682 | CB  | GLN | A | 223 | 25.595 | 42.133 | 22.940 | 1.00 | 34.87 | C |
| ATOM | 1683 | CG  | GLN | A | 223 | 25.364 | 42.825 | 21.599 | 1.00 | 36.55 | C |
| ATOM | 1684 | CD  | GLN | A | 223 | 23.990 | 42.635 | 21.020 | 1.00 | 39.56 | C |
| ATOM | 1685 | OE1 | GLN | A | 223 | 22.986 | 42.824 | 21.701 | 1.00 | 42.40 | O |
| ATOM | 1686 | NE2 | GLN | A | 223 | 23.936 | 42.294 | 19.742 | 1.00 | 41.89 | N |
| ATOM | 1687 | N   | PHE | A | 224 | 28.198 | 42.219 | 25.534 | 1.00 | 34.13 | N |
| ATOM | 1688 | CA  | PHE | A | 224 | 28.437 | 42.270 | 26.965 | 1.00 | 34.17 | C |
| ATOM | 1689 | C   | PHE | A | 224 | 27.941 | 43.571 | 27.570 | 1.00 | 34.88 | C |
| ATOM | 1690 | O   | PHE | A | 224 | 27.310 | 43.549 | 28.622 | 1.00 | 35.50 | O |
| ATOM | 1691 | CB  | PHE | A | 224 | 29.932 | 42.159 | 27.224 | 1.00 | 33.66 | C |
| ATOM | 1692 | CG  | PHE | A | 224 | 30.305 | 42.027 | 28.661 | 1.00 | 32.69 | C |
| ATOM | 1693 | CD1 | PHE | A | 224 | 30.429 | 43.137 | 29.476 | 1.00 | 33.11 | C |
| ATOM | 1694 | CD2 | PHE | A | 224 | 30.609 | 40.790 | 29.191 | 1.00 | 31.85 | C |
| ATOM | 1695 | CE1 | PHE | A | 224 | 30.821 | 43.003 | 30.817 | 1.00 | 31.76 | C |
| ATOM | 1696 | CE2 | PHE | A | 224 | 30.993 | 40.661 | 30.498 | 1.00 | 31.29 | C |
| ATOM | 1697 | CZ  | PHE | A | 224 | 31.098 | 41.775 | 31.316 | 1.00 | 30.73 | C |
| ATOM | 1698 | N   | GLU | A | 225 | 28.235 | 44.706 | 26.930 | 1.00 | 35.46 | N |
| ATOM | 1699 | CA  | GLU | A | 225 | 27.852 | 45.994 | 27.492 | 1.00 | 35.85 | C |
| ATOM | 1700 | C   | GLU | A | 225 | 26.362 | 46.133 | 27.608 | 1.00 | 35.42 | C |
| ATOM | 1701 | O   | GLU | A | 225 | 25.873 | 46.955 | 28.386 | 1.00 | 35.16 | O |
| ATOM | 1702 | CB  | GLU | A | 225 | 28.401 | 47.175 | 26.688 | 1.00 | 36.59 | C |
| ATOM | 1703 | CG  | GLU | A | 225 | 29.892 | 47.377 | 26.917 | 1.00 | 39.78 | C |
| ATOM | 1704 | CD  | GLU | A | 225 | 30.357 | 48.822 | 27.125 | 1.00 | 43.65 | C |
| ATOM | 1705 | OE1 | GLU | A | 225 | 29.937 | 49.524 | 28.099 | 1.00 | 44.64 | O |
| ATOM | 1706 | OE2 | GLU | A | 225 | 31.224 | 49.234 | 26.319 | 1.00 | 47.74 | O |
| ATOM | 1707 | N   | CYS | A | 226 | 25.633 | 45.329 | 26.851 | 1.00 | 35.07 | N |
| ATOM | 1708 | CA  | CYS | A | 226 | 24.192 | 45.453 | 26.842 | 1.00 | 34.93 | C |
| ATOM | 1709 | C   | CYS | A | 226 | 23.473 | 44.498 | 27.770 | 1.00 | 34.91 | C |
| ATOM | 1710 | O   | CYS | A | 226 | 22.266 | 44.654 | 28.019 | 1.00 | 34.86 | O |
| ATOM | 1711 | CB  | CYS | A | 226 | 23.681 | 45.196 | 25.448 | 1.00 | 34.80 | C |
| ATOM | 1712 | SG  | CYS | A | 226 | 24.135 | 46.461 | 24.291 | 1.00 | 34.76 | S |
| ATOM | 1713 | N   | LEU | A | 227 | 24.191 | 43.521 | 28.296 | 1.00 | 34.47 | N |
| ATOM | 1714 | CA  | LEU | A | 227 | 23.509 | 42.483 | 29.025 | 1.00 | 34.57 | C |
| ATOM | 1715 | C   | LEU | A | 227 | 23.815 | 42.408 | 30.503 | 1.00 | 34.08 | C |
| ATOM | 1716 | O   | LEU | A | 227 | 23.122 | 41.725 | 31.235 | 1.00 | 33.57 | O |
| ATOM | 1717 | CB  | LEU | A | 227 | 23.739 | 41.162 | 28.313 | 1.00 | 34.97 | C |
| ATOM | 1718 | CG  | LEU | A | 227 | 22.883 | 41.127 | 27.047 | 1.00 | 36.04 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1719 | CD1 | LEU | A | 227 | 23.454 | 40.177 | 26.043 | 1.00 | 37.99 | C |
| ATOM | 1720 | CD2 | LEU | A | 227 | 21.474 | 40.719 | 27.394 | 1.00 | 36.66 | C |
| ATOM | 1721 | N   | TYR | A | 228 | 24.866 | 43.104 | 30.917 | 1.00 | 34.23 | N |
| ATOM | 1722 | CA  | TYR | A | 228 | 25.172 | 43.334 | 32.329 | 1.00 | 34.02 | C |
| ATOM | 1723 | C   | TYR | A | 228 | 25.163 | 42.091 | 33.196 | 1.00 | 33.81 | C |
| ATOM | 1724 | O   | TYR | A | 228 | 24.294 | 41.900 | 34.041 | 1.00 | 33.87 | O |
| ATOM | 1725 | CB  | TYR | A | 228 | 24.183 | 44.345 | 32.897 | 1.00 | 33.73 | C |
| ATOM | 1726 | CG  | TYR | A | 228 | 24.153 | 45.658 | 32.166 | 1.00 | 33.50 | C |
| ATOM | 1727 | CD1 | TYR | A | 228 | 24.947 | 46.712 | 32.568 | 1.00 | 33.63 | C |
| ATOM | 1728 | CD2 | TYR | A | 228 | 23.312 | 45.853 | 31.086 | 1.00 | 35.03 | C |
| ATOM | 1729 | CE1 | TYR | A | 228 | 24.903 | 47.932 | 31.924 | 1.00 | 34.25 | C |
| ATOM | 1730 | CE2 | TYR | A | 228 | 23.268 | 47.066 | 30.419 | 1.00 | 35.62 | C |
| ATOM | 1731 | CZ  | TYR | A | 228 | 24.068 | 48.106 | 30.848 | 1.00 | 35.60 | C |
| ATOM | 1732 | OH  | TYR | A | 228 | 24.027 | 49.324 | 30.203 | 1.00 | 36.79 | O |
| ATOM | 1733 | N   | PRO | A | 229 | 26.170 | 41.263 | 33.027 | 1.00 | 33.75 | N |
| ATOM | 1734 | CA  | PRO | A | 229 | 26.255 | 40.032 | 33.791 | 1.00 | 33.73 | C |
| ATOM | 1735 | C   | PRO | A | 229 | 26.538 | 40.313 | 35.231 | 1.00 | 33.32 | C |
| ATOM | 1736 | O   | PRO | A | 229 | 27.228 | 41.263 | 35.530 | 1.00 | 33.73 | O |
| ATOM | 1737 | CB  | PRO | A | 229 | 27.449 | 39.319 | 33.169 | 1.00 | 33.87 | C |
| ATOM | 1738 | CG  | PRO | A | 229 | 28.264 | 40.366 | 32.543 | 1.00 | 33.66 | C |
| ATOM | 1739 | CD  | PRO | A | 229 | 27.334 | 41.457 | 32.156 | 1.00 | 34.15 | C |
| ATOM | 1740 | N   | TYR | A | 230 | 25.992 | 39.509 | 36.122 | 1.00 | 32.95 | N |
| ATOM | 1741 | CA  | TYR | A | 230 | 26.330 | 39.654 | 37.510 | 1.00 | 32.64 | C |
| ATOM | 1742 | C   | TYR | A | 230 | 27.836 | 39.534 | 37.651 | 1.00 | 32.59 | C |
| ATOM | 1743 | O   | TYR | A | 230 | 28.536 | 39.020 | 36.793 | 1.00 | 32.76 | O |
| ATOM | 1744 | CB  | TYR | A | 230 | 25.713 | 38.547 | 38.351 | 1.00 | 32.25 | C |
| ATOM | 1745 | CG  | TYR | A | 230 | 24.237 | 38.640 | 38.573 | 1.00 | 31.53 | C |
| ATOM | 1746 | CD1 | TYR | A | 230 | 23.346 | 38.125 | 37.641 | 1.00 | 31.07 | C |
| ATOM | 1747 | CD2 | TYR | A | 230 | 23.727 | 39.192 | 39.748 | 1.00 | 29.93 | C |
| ATOM | 1748 | CE1 | TYR | A | 230 | 21.996 | 38.185 | 37.859 | 1.00 | 31.19 | C |
| ATOM | 1749 | CE2 | TYR | A | 230 | 22.395 | 39.253 | 39.980 | 1.00 | 28.83 | C |
| ATOM | 1750 | CZ  | TYR | A | 230 | 21.523 | 38.755 | 39.040 | 1.00 | 31.04 | C |
| ATOM | 1751 | OH  | TYR | A | 230 | 20.165 | 38.816 | 39.272 | 1.00 | 32.40 | O |
| ATOM | 1752 | N   | PRO | A | 231 | 28.328 | 40.016 | 38.764 | 1.00 | 32.69 | N |
| ATOM | 1753 | CA  | PRO | A | 231 | 29.725 | 39.852 | 39.124 | 1.00 | 32.75 | C |
| ATOM | 1754 | C   | PRO | A | 231 | 30.159 | 38.384 | 39.159 | 1.00 | 32.72 | C |
| ATOM | 1755 | O   | PRO | A | 231 | 29.434 | 37.497 | 39.604 | 1.00 | 32.86 | O |
| ATOM | 1756 | CB  | PRO | A | 231 | 29.768 | 40.423 | 40.533 | 1.00 | 32.82 | C |
| ATOM | 1757 | CG  | PRO | A | 231 | 28.625 | 41.349 | 40.605 | 1.00 | 32.96 | C |
| ATOM | 1758 | CD  | PRO | A | 231 | 27.576 | 40.802 | 39.751 | 1.00 | 32.88 | C |
| ATOM | 1759 | N   | VAL | A | 232 | 31.387 | 38.151 | 38.740 | 1.00 | 32.40 | N |
| ATOM | 1760 | CA  | VAL | A | 232 | 31.938 | 36.825 | 38.680 | 1.00 | 32.10 | C |
| ATOM | 1761 | C   | VAL | A | 232 | 31.776 | 36.022 | 39.963 | 1.00 | 32.41 | C |
| ATOM | 1762 | O   | VAL | A | 232 | 31.546 | 34.826 | 39.906 | 1.00 | 32.96 | O |
| ATOM | 1763 | CB  | VAL | A | 232 | 33.422 | 36.918 | 38.332 | 1.00 | 32.04 | C |
| ATOM | 1764 | CG1 | VAL | A | 232 | 34.131 | 35.666 | 38.721 | 1.00 | 31.82 | C |
| ATOM | 1765 | CG2 | VAL | A | 232 | 33.601 | 37.221 | 36.851 | 1.00 | 31.85 | C |
| ATOM | 1766 | N   | HIS | A | 233 | 31.918 | 36.650 | 41.124 | 1.00 | 32.61 | N |
| ATOM | 1767 | CA  | HIS | A | 233 | 31.819 | 35.910 | 42.376 | 1.00 | 32.41 | C |
| ATOM | 1768 | C   | HIS | A | 233 | 30.383 | 35.727 | 42.874 | 1.00 | 32.27 | C |
| ATOM | 1769 | O   | HIS | A | 233 | 30.134 | 35.052 | 43.860 | 1.00 | 32.05 | O |
| ATOM | 1770 | CB  | HIS | A | 233 | 32.667 | 36.577 | 43.458 | 1.00 | 32.52 | C |
| ATOM | 1771 | CG  | HIS | A | 233 | 34.135 | 36.579 | 43.164 | 1.00 | 33.14 | C |
| ATOM | 1772 | ND1 | HIS | A | 233 | 34.787 | 37.672 | 42.631 | 1.00 | 34.57 | N |
| ATOM | 1773 | CD2 | HIS | A | 233 | 35.083 | 35.629 | 43.342 | 1.00 | 34.15 | C |
| ATOM | 1774 | CE1 | HIS | A | 233 | 36.071 | 37.398 | 42.497 | 1.00 | 34.40 | C |
| ATOM | 1775 | NE2 | HIS | A | 233 | 36.278 | 36.164 | 42.922 | 1.00 | 35.34 | N |
| ATOM | 1776 | N   | HIS | A | 234 | 29.423 | 36.314 | 42.194 | 1.00 | 32.53 | N |
| ATOM | 1777 | CA  | HIS | A | 234 | 28.038 | 36.145 | 42.604 | 1.00 | 33.01 | C |
| ATOM | 1778 | C   | HIS | A | 234 | 27.503 | 34.834 | 42.094 | 1.00 | 33.09 | C |
| ATOM | 1779 | O   | HIS | A | 234 | 27.932 | 34.325 | 41.068 | 1.00 | 33.26 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1780 | CB  | HIS | A | 234 | 27.221 | 37.276 | 42.024 | 1.00 | 33.15 | C |
| ATOM | 1781 | CG  | HIS | A | 234 | 25.817 | 37.383 | 42.531 | 1.00 | 32.96 | C |
| ATOM | 1782 | ND1 | HIS | A | 234 | 24.767 | 36.704 | 41.951 | 1.00 | 32.53 | N |
| ATOM | 1783 | CD2 | HIS | A | 234 | 25.268 | 38.191 | 43.471 | 1.00 | 32.12 | C |
| ATOM | 1784 | CE1 | HIS | A | 234 | 23.639 | 37.056 | 42.540 | 1.00 | 32.45 | C |
| ATOM | 1785 | NE2 | HIS | A | 234 | 23.916 | 37.953 | 43.470 | 1.00 | 32.09 | N |
| ATOM | 1786 | N   | PRO | A | 235 | 26.571 | 34.263 | 42.827 | 1.00 | 33.15 | N |
| ATOM | 1787 | CA  | PRO | A | 235 | 25.985 | 32.996 | 42.410 | 1.00 | 32.79 | C |
| ATOM | 1788 | C   | PRO | A | 235 | 25.386 | 33.045 | 41.026 | 1.00 | 32.62 | C |
| ATOM | 1789 | O   | PRO | A | 235 | 25.210 | 31.990 | 40.440 | 1.00 | 32.65 | O |
| ATOM | 1790 | CB  | PRO | A | 235 | 24.897 | 32.773 | 43.450 | 1.00 | 33.00 | C |
| ATOM | 1791 | CG  | PRO | A | 235 | 25.412 | 33.500 | 44.672 | 1.00 | 32.79 | C |
| ATOM | 1792 | CD  | PRO | A | 235 | 26.049 | 34.725 | 44.128 | 1.00 | 33.00 | C |
| ATOM | 1793 | N   | CYS | A | 236 | 25.095 | 34.226 | 40.493 | 1.00 | 32.39 | N |
| ATOM | 1794 | CA  | CYS | A | 236 | 24.487 | 34.286 | 39.185 | 1.00 | 32.11 | C |
| ATOM | 1795 | C   | CYS | A | 236 | 25.529 | 34.640 | 38.139 | 1.00 | 32.34 | C |
| ATOM | 1796 | O   | CYS | A | 236 | 25.217 | 35.034 | 37.018 | 1.00 | 32.23 | O |
| ATOM | 1797 | CB  | CYS | A | 236 | 23.270 | 35.192 | 39.206 | 1.00 | 32.02 | C |
| ATOM | 1798 | SG  | CYS | A | 236 | 21.990 | 34.545 | 40.326 | 1.00 | 32.09 | S |
| ATOM | 1799 | N   | ASP | A | 237 | 26.789 | 34.456 | 38.511 | 1.00 | 32.71 | N |
| ATOM | 1800 | CA  | ASP | A | 237 | 27.883 | 34.609 | 37.576 | 1.00 | 33.21 | C |
| ATOM | 1801 | C   | ASP | A | 237 | 27.518 | 34.022 | 36.211 | 1.00 | 33.63 | C |
| ATOM | 1802 | O   | ASP | A | 237 | 27.042 | 32.911 | 36.095 | 1.00 | 33.33 | O |
| ATOM | 1803 | CB  | ASP | A | 237 | 29.139 | 33.964 | 38.132 | 1.00 | 33.01 | C |
| ATOM | 1804 | CG  | ASP | A | 237 | 30.283 | 33.981 | 37.151 | 1.00 | 33.76 | C |
| ATOM | 1805 | OD1 | ASP | A | 237 | 30.340 | 34.874 | 36.279 | 1.00 | 34.52 | O |
| ATOM | 1806 | OD2 | ASP | A | 237 | 31.193 | 33.135 | 37.181 | 1.00 | 36.09 | O |
| ATOM | 1807 | N   | ARG | A | 238 | 27.731 | 34.821 | 35.180 | 1.00 | 34.68 | N |
| ATOM | 1808 | CA  | ARG | A | 238 | 27.414 | 34.451 | 33.810 | 1.00 | 35.15 | C |
| ATOM | 1809 | C   | ARG | A | 238 | 25.962 | 34.690 | 33.375 | 1.00 | 34.98 | C |
| ATOM | 1810 | O   | ARG | A | 238 | 25.664 | 34.543 | 32.197 | 1.00 | 34.26 | O |
| ATOM | 1811 | CB  | ARG | A | 238 | 27.819 | 33.020 | 33.561 | 1.00 | 35.64 | C |
| ATOM | 1812 | CG  | ARG | A | 238 | 29.286 | 32.847 | 33.620 | 1.00 | 36.86 | C |
| ATOM | 1813 | CD  | ARG | A | 238 | 29.682 | 31.474 | 33.268 | 1.00 | 38.59 | C |
| ATOM | 1814 | NE  | ARG | A | 238 | 29.321 | 30.549 | 34.338 | 1.00 | 41.64 | N |
| ATOM | 1815 | CZ  | ARG | A | 238 | 28.265 | 29.755 | 34.286 | 1.00 | 43.17 | C |
| ATOM | 1816 | NH1 | ARG | A | 238 | 27.459 | 29.802 | 33.218 | 1.00 | 44.38 | N |
| ATOM | 1817 | NH2 | ARG | A | 238 | 28.006 | 28.923 | 35.291 | 1.00 | 42.18 | N |
| ATOM | 1818 | N   | GLN | A | 239 | 25.067 | 35.044 | 34.303 | 1.00 | 35.13 | N |
| ATOM | 1819 | CA  | GLN | A | 239 | 23.683 | 35.360 | 33.920 | 1.00 | 35.13 | C |
| ATOM | 1820 | C   | GLN | A | 239 | 23.558 | 36.872 | 33.825 | 1.00 | 34.56 | C |
| ATOM | 1821 | O   | GLN | A | 239 | 24.240 | 37.587 | 34.539 | 1.00 | 34.65 | O |
| ATOM | 1822 | CB  | GLN | A | 239 | 22.646 | 34.839 | 34.921 | 1.00 | 35.27 | C |
| ATOM | 1823 | CG  | GLN | A | 239 | 22.952 | 33.510 | 35.566 | 1.00 | 37.30 | C |
| ATOM | 1824 | CD  | GLN | A | 239 | 23.270 | 32.431 | 34.552 | 1.00 | 41.59 | C |
| ATOM | 1825 | OE1 | GLN | A | 239 | 22.418 | 32.072 | 33.726 | 1.00 | 45.42 | O |
| ATOM | 1826 | NE2 | GLN | A | 239 | 24.491 | 31.899 | 34.609 | 1.00 | 42.92 | N |
| ATOM | 1827 | N   | SER | A | 240 | 22.705 | 37.358 | 32.930 | 1.00 | 33.99 | N |
| ATOM | 1828 | CA  | SER | A | 240 | 22.455 | 38.785 | 32.802 | 1.00 | 33.14 | C |
| ATOM | 1829 | C   | SER | A | 240 | 21.613 | 39.254 | 33.957 | 1.00 | 32.53 | C |
| ATOM | 1830 | O   | SER | A | 240 | 20.773 | 38.528 | 34.446 | 1.00 | 31.77 | O |
| ATOM | 1831 | CB  | SER | A | 240 | 21.663 | 39.077 | 31.542 | 1.00 | 33.15 | C |
| ATOM | 1832 | OG  | SER | A | 240 | 20.971 | 40.309 | 31.668 | 1.00 | 33.28 | O |
| ATOM | 1833 | N   | GLN | A | 241 | 21.805 | 40.492 | 34.371 | 1.00 | 32.52 | N |
| ATOM | 1834 | CA  | GLN | A | 241 | 21.022 | 41.025 | 35.476 | 1.00 | 32.54 | C |
| ATOM | 1835 | C   | GLN | A | 241 | 19.711 | 41.629 | 35.001 | 1.00 | 32.44 | C |
| ATOM | 1836 | O   | GLN | A | 241 | 18.872 | 42.019 | 35.804 | 1.00 | 32.16 | O |
| ATOM | 1837 | CB  | GLN | A | 241 | 21.791 | 42.116 | 36.196 | 1.00 | 32.36 | C |
| ATOM | 1838 | CG  | GLN | A | 241 | 22.995 | 41.669 | 36.917 | 1.00 | 32.74 | C |
| ATOM | 1839 | CD  | GLN | A | 241 | 23.760 | 42.837 | 37.450 | 1.00 | 33.65 | C |
| ATOM | 1840 | OE1 | GLN | A | 241 | 23.353 | 43.442 | 38.428 | 1.00 | 34.26 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1841 | NE2 | GLN | A | 241 | 24.858 | 43.182 | 36.794 | 1.00 | 35.62 | N |
| ATOM | 1842 | N   | VAL | A | 242 | 19.513 | 41.708 | 33.705 | 1.00 | 32.07 | N |
| ATOM | 1843 | CA  | VAL | A | 242 | 18.357 | 42.412 | 33.255 | 1.00 | 32.29 | C |
| ATOM | 1844 | C   | VAL | A | 242 | 17.162 | 41.521 | 33.265 | 1.00 | 31.93 | C |
| ATOM | 1845 | O   | VAL | A | 242 | 17.221 | 40.442 | 32.734 | 1.00 | 32.93 | O |
| ATOM | 1846 | CB  | VAL | A | 242 | 18.516 | 42.848 | 31.808 | 1.00 | 32.63 | C |
| ATOM | 1847 | CG1 | VAL | A | 242 | 17.252 | 43.532 | 31.320 | 1.00 | 32.50 | C |
| ATOM | 1848 | CG2 | VAL | A | 242 | 19.717 | 43.714 | 31.655 | 1.00 | 33.06 | C |
| ATOM | 1849 | N   | ASP | A | 243 | 16.067 | 41.977 | 33.838 | 1.00 | 31.76 | N |
| ATOM | 1850 | CA  | ASP | A | 243 | 14.812 | 41.271 | 33.714 | 1.00 | 31.73 | C |
| ATOM | 1851 | C   | ASP | A | 243 | 14.177 | 41.559 | 32.346 | 1.00 | 31.87 | C |
| ATOM | 1852 | O   | ASP | A | 243 | 13.536 | 42.595 | 32.150 | 1.00 | 31.46 | O |
| ATOM | 1853 | CB  | ASP | A | 243 | 13.861 | 41.689 | 34.830 | 1.00 | 31.61 | C |
| ATOM | 1854 | CG  | ASP | A | 243 | 12.488 | 41.049 | 34.708 | 1.00 | 32.08 | C |
| ATOM | 1855 | OD1 | ASP | A | 243 | 12.164 | 40.448 | 33.655 | 1.00 | 30.69 | O |
| ATOM | 1856 | OD2 | ASP | A | 243 | 11.654 | 41.103 | 35.635 | 1.00 | 33.90 | O |
| ATOM | 1857 | N   | PHE | A | 244 | 14.326 | 40.623 | 31.410 | 1.00 | 32.16 | N |
| ATOM | 1858 | CA  | PHE | A | 244 | 13.746 | 40.787 | 30.075 | 1.00 | 32.29 | C |
| ATOM | 1859 | C   | PHE | A | 244 | 12.252 | 41.087 | 30.092 | 1.00 | 32.74 | C |
| ATOM | 1860 | O   | PHE | A | 244 | 11.741 | 41.694 | 29.162 | 1.00 | 32.51 | O |
| ATOM | 1861 | CB  | PHE | A | 244 | 13.963 | 39.559 | 29.220 | 1.00 | 31.99 | C |
| ATOM | 1862 | CG  | PHE | A | 244 | 15.327 | 39.446 | 28.650 | 1.00 | 31.29 | C |
| ATOM | 1863 | CD1 | PHE | A | 244 | 16.436 | 39.886 | 29.342 | 1.00 | 31.05 | C |
| ATOM | 1864 | CD2 | PHE | A | 244 | 15.500 | 38.861 | 27.421 | 1.00 | 31.04 | C |
| ATOM | 1865 | CE1 | PHE | A | 244 | 17.684 | 39.733 | 28.815 | 1.00 | 31.37 | C |
| ATOM | 1866 | CE2 | PHE | A | 244 | 16.742 | 38.709 | 26.888 | 1.00 | 31.39 | C |
| ATOM | 1867 | CZ  | PHE | A | 244 | 17.839 | 39.141 | 27.584 | 1.00 | 31.77 | C |
| ATOM | 1868 | N   | ASP | A | 245 | 11.547 | 40.646 | 31.124 | 1.00 | 33.52 | N |
| ATOM | 1869 | CA  | ASP | A | 245 | 10.130 | 40.946 | 31.214 | 1.00 | 34.33 | C |
| ATOM | 1870 | C   | ASP | A | 245 | 9.831  | 42.375 | 31.606 | 1.00 | 34.52 | C |
| ATOM | 1871 | O   | ASP | A | 245 | 8.789  | 42.902 | 31.251 | 1.00 | 34.40 | O |
| ATOM | 1872 | CB  | ASP | A | 245 | 9.448  | 40.015 | 32.188 | 1.00 | 34.59 | C |
| ATOM | 1873 | CG  | ASP | A | 245 | 9.361  | 38.639 | 31.658 | 1.00 | 35.47 | C |
| ATOM | 1874 | OD1 | ASP | A | 245 | 9.282  | 38.519 | 30.420 | 1.00 | 36.40 | O |
| ATOM | 1875 | OD2 | ASP | A | 245 | 9.384  | 37.624 | 32.383 | 1.00 | 37.65 | O |
| ATOM | 1876 | N   | ASN | A | 246 | 10.737 | 43.000 | 32.339 | 1.00 | 35.03 | N |
| ATOM | 1877 | CA  | ASN | A | 246 | 10.531 | 44.364 | 32.776 | 1.00 | 35.38 | C |
| ATOM | 1878 | C   | ASN | A | 246 | 11.873 | 45.003 | 32.896 | 1.00 | 34.97 | C |
| ATOM | 1879 | O   | ASN | A | 246 | 12.370 | 45.160 | 33.994 | 1.00 | 35.01 | O |
| ATOM | 1880 | CB  | ASN | A | 246 | 9.843  | 44.397 | 34.136 | 1.00 | 35.69 | C |
| ATOM | 1881 | CG  | ASN | A | 246 | 9.395  | 45.800 | 34.533 | 1.00 | 37.41 | C |
| ATOM | 1882 | OD1 | ASN | A | 246 | 9.241  | 46.691 | 33.682 | 1.00 | 38.99 | O |
| ATOM | 1883 | ND2 | ASN | A | 246 | 9.186  | 46.006 | 35.836 | 1.00 | 38.90 | N |
| ATOM | 1884 | N   | PRO | A | 247 | 12.468 | 45.357 | 31.766 | 1.00 | 34.87 | N |
| ATOM | 1885 | CA  | PRO | A | 247 | 13.816 | 45.931 | 31.766 | 1.00 | 34.87 | C |
| ATOM | 1886 | C   | PRO | A | 247 | 13.868 | 47.295 | 32.407 | 1.00 | 34.83 | C |
| ATOM | 1887 | O   | PRO | A | 247 | 13.038 | 48.159 | 32.127 | 1.00 | 34.82 | O |
| ATOM | 1888 | CB  | PRO | A | 247 | 14.184 | 46.046 | 30.288 | 1.00 | 34.75 | C |
| ATOM | 1889 | CG  | PRO | A | 247 | 13.028 | 45.475 | 29.507 | 1.00 | 34.95 | C |
| ATOM | 1890 | CD  | PRO | A | 247 | 11.892 | 45.241 | 30.419 | 1.00 | 34.75 | C |
| ATOM | 1891 | N   | ASP | A | 248 | 14.861 | 47.448 | 33.270 | 1.00 | 34.67 | N |
| ATOM | 1892 | CA  | ASP | A | 248 | 15.112 | 48.654 | 34.003 | 1.00 | 34.76 | C |
| ATOM | 1893 | C   | ASP | A | 248 | 16.205 | 49.419 | 33.294 | 1.00 | 34.89 | C |
| ATOM | 1894 | O   | ASP | A | 248 | 17.395 | 49.240 | 33.568 | 1.00 | 34.59 | O |
| ATOM | 1895 | CB  | ASP | A | 248 | 15.583 | 48.265 | 35.387 | 1.00 | 34.87 | C |
| ATOM | 1896 | CG  | ASP | A | 248 | 15.703 | 49.433 | 36.329 | 1.00 | 35.10 | C |
| ATOM | 1897 | OD1 | ASP | A | 248 | 15.958 | 50.583 | 35.902 | 1.00 | 34.24 | O |
| ATOM | 1898 | OD2 | ASP | A | 248 | 15.574 | 49.259 | 37.550 | 1.00 | 36.72 | O |
| ATOM | 1899 | N   | TYR | A | 249 | 15.793 | 50.302 | 32.399 | 1.00 | 35.08 | N |
| ATOM | 1900 | CA  | TYR | A | 249 | 16.743 | 51.063 | 31.615 | 1.00 | 35.24 | C |
| ATOM | 1901 | C   | TYR | A | 249 | 17.578 | 52.071 | 32.400 | 1.00 | 35.48 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1902 | O   | TYR | A | 249 | 18.570 | 52.567 | 31.880 | 1.00 | 35.44 | O |
| ATOM | 1903 | CB  | TYR | A | 249 | 16.021 | 51.741 | 30.465 | 1.00 | 35.05 | C |
| ATOM | 1904 | CG  | TYR | A | 249 | 15.304 | 50.761 | 29.586 | 1.00 | 34.41 | C |
| ATOM | 1905 | CD1 | TYR | A | 249 | 15.977 | 49.718 | 28.971 | 1.00 | 34.17 | C |
| ATOM | 1906 | CD2 | TYR | A | 249 | 13.955 | 50.865 | 29.383 | 1.00 | 34.14 | C |
| ATOM | 1907 | CE1 | TYR | A | 249 | 15.312 | 48.828 | 28.172 | 1.00 | 33.95 | C |
| ATOM | 1908 | CE2 | TYR | A | 249 | 13.287 | 49.983 | 28.595 | 1.00 | 33.71 | C |
| ATOM | 1909 | CZ  | TYR | A | 249 | 13.954 | 48.974 | 27.989 | 1.00 | 34.19 | C |
| ATOM | 1910 | OH  | TYR | A | 249 | 13.232 | 48.113 | 27.194 | 1.00 | 35.64 | O |
| ATOM | 1911 | N   | GLU | A | 250 | 17.207 | 52.393 | 33.631 | 1.00 | 35.82 | N |
| ATOM | 1912 | CA  | GLU | A | 250 | 18.072 | 53.273 | 34.399 | 1.00 | 36.69 | C |
| ATOM | 1913 | C   | GLU | A | 250 | 19.331 | 52.562 | 34.834 | 1.00 | 36.69 | C |
| ATOM | 1914 | O   | GLU | A | 250 | 20.424 | 53.102 | 34.715 | 1.00 | 36.84 | O |
| ATOM | 1915 | CB  | GLU | A | 250 | 17.369 | 53.836 | 35.607 | 1.00 | 37.10 | C |
| ATOM | 1916 | CG  | GLU | A | 250 | 16.173 | 54.653 | 35.195 | 1.00 | 39.48 | C |
| ATOM | 1917 | CD  | GLU | A | 250 | 15.559 | 55.362 | 36.359 | 1.00 | 42.67 | C |
| ATOM | 1918 | OE1 | GLU | A | 250 | 16.128 | 55.258 | 37.469 | 1.00 | 45.95 | O |
| ATOM | 1919 | OE2 | GLU | A | 250 | 14.529 | 56.030 | 36.160 | 1.00 | 44.93 | O |
| ATOM | 1920 | N   | ARG | A | 251 | 19.202 | 51.344 | 35.332 | 1.00 | 36.55 | N |
| ATOM | 1921 | CA  | ARG | A | 251 | 20.389 | 50.666 | 35.773 | 1.00 | 36.36 | C |
| ATOM | 1922 | C   | ARG | A | 251 | 21.124 | 50.162 | 34.584 | 1.00 | 35.91 | C |
| ATOM | 1923 | O   | ARG | A | 251 | 22.347 | 50.117 | 34.588 | 1.00 | 36.89 | O |
| ATOM | 1924 | CB  | ARG | A | 251 | 20.062 | 49.495 | 36.697 | 1.00 | 36.66 | C |
| ATOM | 1925 | CG  | ARG | A | 251 | 19.329 | 49.936 | 37.981 | 1.00 | 38.10 | C |
| ATOM | 1926 | CD  | ARG | A | 251 | 18.848 | 48.824 | 38.916 | 1.00 | 39.00 | C |
| ATOM | 1927 | NE  | ARG | A | 251 | 19.969 | 48.005 | 39.371 | 1.00 | 40.55 | N |
| ATOM | 1928 | CZ  | ARG | A | 251 | 19.895 | 46.712 | 39.648 | 1.00 | 41.33 | C |
| ATOM | 1929 | NH1 | ARG | A | 251 | 18.742 | 46.068 | 39.542 | 1.00 | 42.58 | N |
| ATOM | 1930 | NH2 | ARG | A | 251 | 20.978 | 46.058 | 40.025 | 1.00 | 41.49 | N |
| ATOM | 1931 | N   | PHE | A | 252 | 20.388 | 49.807 | 33.545 | 1.00 | 35.06 | N |
| ATOM | 1932 | CA  | PHE | A | 252 | 20.988 | 49.065 | 32.455 | 1.00 | 34.37 | C |
| ATOM | 1933 | C   | PHE | A | 252 | 20.653 | 49.675 | 31.138 | 1.00 | 33.82 | C |
| ATOM | 1934 | O   | PHE | A | 252 | 20.048 | 49.042 | 30.278 | 1.00 | 33.57 | O |
| ATOM | 1935 | CB  | PHE | A | 252 | 20.429 | 47.662 | 32.458 | 1.00 | 34.19 | C |
| ATOM | 1936 | CG  | PHE | A | 252 | 20.404 | 47.019 | 33.803 | 1.00 | 33.98 | C |
| ATOM | 1937 | CD1 | PHE | A | 252 | 21.559 | 46.855 | 34.532 | 1.00 | 33.98 | C |
| ATOM | 1938 | CD2 | PHE | A | 252 | 19.220 | 46.560 | 34.337 | 1.00 | 32.84 | C |
| ATOM | 1939 | CE1 | PHE | A | 252 | 21.519 | 46.238 | 35.760 | 1.00 | 33.51 | C |
| ATOM | 1940 | CE2 | PHE | A | 252 | 19.189 | 45.953 | 35.560 | 1.00 | 32.14 | C |
| ATOM | 1941 | CZ  | PHE | A | 252 | 20.327 | 45.789 | 36.269 | 1.00 | 31.96 | C |
| ATOM | 1942 | N   | PRO | A | 253 | 21.087 | 50.903 | 30.959 | 1.00 | 33.27 | N |
| ATOM | 1943 | CA  | PRO | A | 253 | 20.677 | 51.675 | 29.795 | 1.00 | 32.92 | C |
| ATOM | 1944 | C   | PRO | A | 253 | 21.008 | 50.995 | 28.470 | 1.00 | 32.86 | C |
| ATOM | 1945 | O   | PRO | A | 253 | 20.215 | 51.136 | 27.541 | 1.00 | 32.58 | O |
| ATOM | 1946 | CB  | PRO | A | 253 | 21.464 | 52.957 | 29.962 | 1.00 | 32.58 | C |
| ATOM | 1947 | CG  | PRO | A | 253 | 22.584 | 52.562 | 30.808 | 1.00 | 32.44 | C |
| ATOM | 1948 | CD  | PRO | A | 253 | 22.038 | 51.640 | 31.802 | 1.00 | 32.67 | C |
| ATOM | 1949 | N   | ASN | A | 254 | 22.108 | 50.253 | 28.359 | 1.00 | 32.60 | N |
| ATOM | 1950 | CA  | ASN | A | 254 | 22.419 | 49.726 | 27.037 | 1.00 | 32.87 | C |
| ATOM | 1951 | C   | ASN | A | 254 | 21.564 | 48.569 | 26.615 | 1.00 | 32.59 | C |
| ATOM | 1952 | O   | ASN | A | 254 | 21.671 | 48.088 | 25.503 | 1.00 | 32.69 | O |
| ATOM | 1953 | CB  | ASN | A | 254 | 23.892 | 49.414 | 26.852 | 1.00 | 32.72 | C |
| ATOM | 1954 | CG  | ASN | A | 254 | 24.710 | 50.665 | 26.745 | 1.00 | 33.92 | C |
| ATOM | 1955 | OD1 | ASN | A | 254 | 25.428 | 51.022 | 27.672 | 1.00 | 37.05 | O |
| ATOM | 1956 | ND2 | ASN | A | 254 | 24.569 | 51.380 | 25.626 | 1.00 | 34.86 | N |
| ATOM | 1957 | N   | PHE | A | 255 | 20.690 | 48.124 | 27.491 | 1.00 | 32.37 | N |
| ATOM | 1958 | CA  | PHE | A | 255 | 19.834 | 47.057 | 27.101 | 1.00 | 32.19 | C |
| ATOM | 1959 | C   | PHE | A | 255 | 18.932 | 47.578 | 26.006 | 1.00 | 32.36 | C |
| ATOM | 1960 | O   | PHE | A | 255 | 18.267 | 46.819 | 25.326 | 1.00 | 32.64 | O |
| ATOM | 1961 | CB  | PHE | A | 255 | 18.990 | 46.572 | 28.250 | 1.00 | 31.93 | C |
| ATOM | 1962 | CG  | PHE | A | 255 | 18.249 | 45.354 | 27.918 | 1.00 | 31.43 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1963 | CD1 | PHE | A | 255 | 18.919 | 44.176 | 27.718 | 1.00 | 33.75 | C |
| ATOM | 1964 | CD2 | PHE | A | 255 | 16.909 | 45.392 | 27.718 | 1.00 | 31.23 | C |
| ATOM | 1965 | CE1 | PHE | A | 255 | 18.239 | 43.035 | 27.367 | 1.00 | 34.05 | C |
| ATOM | 1966 | CE2 | PHE | A | 255 | 16.230 | 44.275 | 27.380 | 1.00 | 32.00 | C |
| ATOM | 1967 | CZ  | PHE | A | 255 | 16.890 | 43.088 | 27.203 | 1.00 | 32.84 | C |
| ATOM | 1968 | N   | GLN | A | 256 | 18.890 | 48.888 | 25.844 | 1.00 | 32.46 | N |
| ATOM | 1969 | CA  | GLN | A | 256 | 18.078 | 49.456 | 24.794 | 1.00 | 32.37 | C |
| ATOM | 1970 | C   | GLN | A | 256 | 18.776 | 49.342 | 23.455 | 1.00 | 32.34 | C |
| ATOM | 1971 | O   | GLN | A | 256 | 18.260 | 49.815 | 22.470 | 1.00 | 32.11 | O |
| ATOM | 1972 | CB  | GLN | A | 256 | 17.777 | 50.924 | 25.061 | 1.00 | 32.28 | C |
| ATOM | 1973 | CG  | GLN | A | 256 | 16.775 | 51.169 | 26.144 | 1.00 | 32.39 | C |
| ATOM | 1974 | CD  | GLN | A | 256 | 16.823 | 52.594 | 26.645 | 1.00 | 32.91 | C |
| ATOM | 1975 | OE1 | GLN | A | 256 | 15.830 | 53.303 | 26.588 | 1.00 | 34.66 | O |
| ATOM | 1976 | NE2 | GLN | A | 256 | 17.982 | 53.021 | 27.125 | 1.00 | 32.30 | N |
| ATOM | 1977 | N   | ASN | A | 257 | 19.956 | 48.744 | 23.404 | 1.00 | 32.78 | N |
| ATOM | 1978 | CA  | ASN | A | 257 | 20.634 | 48.617 | 22.126 | 1.00 | 33.17 | C |
| ATOM | 1979 | C   | ASN | A | 257 | 20.828 | 47.159 | 21.763 | 1.00 | 34.01 | C |
| ATOM | 1980 | O   | ASN | A | 257 | 21.406 | 46.841 | 20.721 | 1.00 | 34.41 | O |
| ATOM | 1981 | CB  | ASN | A | 257 | 21.998 | 49.310 | 22.140 | 1.00 | 32.88 | C |
| ATOM | 1982 | CG  | ASN | A | 257 | 21.928 | 50.750 | 22.595 | 1.00 | 31.31 | C |
| ATOM | 1983 | OD1 | ASN | A | 257 | 22.471 | 51.105 | 23.639 | 1.00 | 27.26 | O |
| ATOM | 1984 | ND2 | ASN | A | 257 | 21.283 | 51.595 | 21.797 | 1.00 | 29.34 | N |
| ATOM | 1985 | N   | VAL | A | 258 | 20.338 | 46.263 | 22.606 | 1.00 | 34.66 | N |
| ATOM | 1986 | CA  | VAL | A | 258 | 20.565 | 44.855 | 22.370 | 1.00 | 35.33 | C |
| ATOM | 1987 | C   | VAL | A | 258 | 19.832 | 44.361 | 21.130 | 1.00 | 35.37 | C |
| ATOM | 1988 | O   | VAL | A | 258 | 18.751 | 44.832 | 20.813 | 1.00 | 34.96 | O |
| ATOM | 1989 | CB  | VAL | A | 258 | 20.144 | 44.010 | 23.558 | 1.00 | 35.59 | C |
| ATOM | 1990 | CG1 | VAL | A | 258 | 18.632 | 43.851 | 23.604 | 1.00 | 35.73 | C |
| ATOM | 1991 | CG2 | VAL | A | 258 | 20.780 | 42.662 | 23.428 | 1.00 | 36.60 | C |
| ATOM | 1992 | N   | VAL | A | 259 | 20.447 | 43.418 | 20.428 | 1.00 | 35.87 | N |
| ATOM | 1993 | CA  | VAL | A | 259 | 19.853 | 42.844 | 19.230 | 1.00 | 36.40 | C |
| ATOM | 1994 | C   | VAL | A | 259 | 20.125 | 41.355 | 19.148 | 1.00 | 36.66 | C |
| ATOM | 1995 | O   | VAL | A | 259 | 21.282 | 40.943 | 19.102 | 1.00 | 36.47 | O |
| ATOM | 1996 | CB  | VAL | A | 259 | 20.450 | 43.459 | 17.969 | 1.00 | 36.47 | C |
| ATOM | 1997 | CG1 | VAL | A | 259 | 19.830 | 42.822 | 16.764 | 1.00 | 36.75 | C |
| ATOM | 1998 | CG2 | VAL | A | 259 | 20.212 | 44.931 | 17.932 | 1.00 | 36.66 | C |
| ATOM | 1999 | N   | GLY | A | 260 | 19.066 | 40.551 | 19.085 | 1.00 | 37.15 | N |
| ATOM | 2000 | CA  | GLY | A | 260 | 19.215 | 39.096 | 19.067 | 1.00 | 37.50 | C |
| ATOM | 2001 | C   | GLY | A | 260 | 19.132 | 38.328 | 17.745 | 1.00 | 37.55 | C |
| ATOM | 2002 | O   | GLY | A | 260 | 18.716 | 38.839 | 16.704 | 1.00 | 37.45 | O |
| ATOM | 2003 | N   | TYR | A | 261 | 19.578 | 37.079 | 17.817 | 1.00 | 37.54 | N |
| ATOM | 2004 | CA  | TYR | A | 261 | 19.466 | 36.113 | 16.744 | 1.00 | 37.52 | C |
| ATOM | 2005 | C   | TYR | A | 261 | 18.530 | 35.107 | 17.358 | 1.00 | 37.09 | C |
| ATOM | 2006 | O   | TYR | A | 261 | 18.788 | 34.648 | 18.466 | 1.00 | 37.12 | O |
| ATOM | 2007 | CB  | TYR | A | 261 | 20.796 | 35.429 | 16.481 | 1.00 | 37.79 | C |
| ATOM | 2008 | CG  | TYR | A | 261 | 21.838 | 36.327 | 15.874 | 1.00 | 39.43 | C |
| ATOM | 2009 | CD1 | TYR | A | 261 | 22.005 | 36.380 | 14.507 | 1.00 | 41.03 | C |
| ATOM | 2010 | CD2 | TYR | A | 261 | 22.648 | 37.125 | 16.662 | 1.00 | 41.07 | C |
| ATOM | 2011 | CE1 | TYR | A | 261 | 22.937 | 37.193 | 13.940 | 1.00 | 41.71 | C |
| ATOM | 2012 | CE2 | TYR | A | 261 | 23.593 | 37.938 | 16.093 | 1.00 | 41.99 | C |
| ATOM | 2013 | CZ  | TYR | A | 261 | 23.725 | 37.960 | 14.728 | 1.00 | 42.45 | C |
| ATOM | 2014 | OH  | TYR | A | 261 | 24.650 | 38.762 | 14.121 | 1.00 | 46.29 | O |
| ATOM | 2015 | N   | GLU | A | 262 | 17.430 | 34.773 | 16.699 | 1.00 | 36.56 | N |
| ATOM | 2016 | CA  | GLU | A | 262 | 16.500 | 33.866 | 17.346 | 1.00 | 35.87 | C |
| ATOM | 2017 | C   | GLU | A | 262 | 16.064 | 32.737 | 16.447 | 1.00 | 35.41 | C |
| ATOM | 2018 | O   | GLU | A | 262 | 16.310 | 32.747 | 15.248 | 1.00 | 35.03 | O |
| ATOM | 2019 | CB  | GLU | A | 262 | 15.320 | 34.639 | 17.943 | 1.00 | 35.67 | C |
| ATOM | 2020 | CG  | GLU | A | 262 | 14.085 | 34.789 | 17.098 | 1.00 | 35.22 | C |
| ATOM | 2021 | CD  | GLU | A | 262 | 13.039 | 35.601 | 17.821 | 1.00 | 35.62 | C |
| ATOM | 2022 | OE1 | GLU | A | 262 | 13.201 | 36.833 | 17.866 | 1.00 | 38.15 | O |
| ATOM | 2023 | OE2 | GLU | A | 262 | 12.074 | 35.031 | 18.367 | 1.00 | 35.12 | O |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2024 | N   | THR | A | 263 | 15.440 | 31.744 | 17.060 | 1.00 | 35.07 | N |
| ATOM | 2025 | CA  | THR | A | 263 | 15.004 | 30.565 | 16.351 | 1.00 | 34.84 | C |
| ATOM | 2026 | C   | THR | A | 263 | 14.138 | 29.670 | 17.224 | 1.00 | 34.38 | C |
| ATOM | 2027 | O   | THR | A | 263 | 14.152 | 29.745 | 18.452 | 1.00 | 34.07 | O |
| ATOM | 2028 | CB  | THR | A | 263 | 16.235 | 29.767 | 15.847 | 1.00 | 34.75 | C |
| ATOM | 2029 | OG1 | THR | A | 263 | 15.864 | 28.964 | 14.731 | 1.00 | 35.81 | O |
| ATOM | 2030 | CG2 | THR | A | 263 | 16.693 | 28.745 | 16.837 | 1.00 | 34.59 | C |
| ATOM | 2031 | N   | VAL | A | 264 | 13.368 | 28.820 | 16.573 | 1.00 | 34.02 | N |
| ATOM | 2032 | CA  | VAL | A | 264 | 12.597 | 27.854 | 17.306 | 1.00 | 33.95 | C |
| ATOM | 2033 | C   | VAL | A | 264 | 13.054 | 26.460 | 16.918 | 1.00 | 33.60 | C |
| ATOM | 2034 | O   | VAL | A | 264 | 12.957 | 26.065 | 15.762 | 1.00 | 33.27 | O |
| ATOM | 2035 | CB  | VAL | A | 264 | 11.112 | 28.019 | 17.075 | 1.00 | 33.95 | C |
| ATOM | 2036 | CG1 | VAL | A | 264 | 10.393 | 26.788 | 17.568 | 1.00 | 34.24 | C |
| ATOM | 2037 | CG2 | VAL | A | 264 | 10.615 | 29.247 | 17.823 | 1.00 | 33.85 | C |
| ATOM | 2038 | N   | VAL | A | 265 | 13.572 | 25.708 | 17.880 | 1.00 | 33.43 | N |
| ATOM | 2039 | CA  | VAL | A | 265 | 13.984 | 24.354 | 17.546 | 1.00 | 33.48 | C |
| ATOM | 2040 | C   | VAL | A | 265 | 12.949 | 23.321 | 17.907 | 1.00 | 32.85 | C |
| ATOM | 2041 | O   | VAL | A | 265 | 12.234 | 23.441 | 18.884 | 1.00 | 32.91 | O |
| ATOM | 2042 | CB  | VAL | A | 265 | 15.332 | 23.954 | 18.139 | 1.00 | 33.61 | C |
| ATOM | 2043 | CG1 | VAL | A | 265 | 16.408 | 24.721 | 17.432 | 1.00 | 34.56 | C |
| ATOM | 2044 | CG2 | VAL | A | 265 | 15.381 | 24.153 | 19.636 | 1.00 | 33.15 | C |
| ATOM | 2045 | N   | GLY | A | 266 | 12.848 | 22.321 | 17.064 | 1.00 | 32.32 | N |
| ATOM | 2046 | CA  | GLY | A | 266 | 11.938 | 21.240 | 17.331 | 1.00 | 32.27 | C |
| ATOM | 2047 | C   | GLY | A | 266 | 12.634 | 19.905 | 17.310 | 1.00 | 31.78 | C |
| ATOM | 2048 | O   | GLY | A | 266 | 13.852 | 19.799 | 17.124 | 1.00 | 31.15 | O |
| ATOM | 2049 | N   | PRO | A | 267 | 11.827 | 18.872 | 17.454 | 1.00 | 31.56 | N |
| ATOM | 2050 | CA  | PRO | A | 267 | 12.343 | 17.516 | 17.547 | 1.00 | 31.40 | C |
| ATOM | 2051 | C   | PRO | A | 267 | 13.203 | 17.314 | 16.336 | 1.00 | 31.22 | C |
| ATOM | 2052 | O   | PRO | A | 267 | 12.755 | 17.631 | 15.241 | 1.00 | 31.24 | O |
| ATOM | 2053 | CB  | PRO | A | 267 | 11.074 | 16.664 | 17.552 | 1.00 | 30.81 | C |
| ATOM | 2054 | CG  | PRO | A | 267 | 10.048 | 17.568 | 18.087 | 1.00 | 31.26 | C |
| ATOM | 2055 | CD  | PRO | A | 267 | 10.358 | 18.900 | 17.451 | 1.00 | 31.85 | C |
| ATOM | 2056 | N   | GLY | A | 268 | 14.445 | 16.891 | 16.536 | 1.00 | 31.06 | N |
| ATOM | 2057 | CA  | GLY | A | 268 | 15.334 | 16.620 | 15.426 | 1.00 | 31.07 | C |
| ATOM | 2058 | C   | GLY | A | 268 | 16.337 | 17.703 | 15.112 | 1.00 | 31.31 | C |
| ATOM | 2059 | O   | GLY | A | 268 | 17.352 | 17.425 | 14.493 | 1.00 | 31.12 | O |
| ATOM | 2060 | N   | ASP | A | 269 | 16.061 | 18.939 | 15.517 | 1.00 | 31.87 | N |
| ATOM | 2061 | CA  | ASP | A | 269 | 16.975 | 20.032 | 15.253 | 1.00 | 32.18 | C |
| ATOM | 2062 | C   | ASP | A | 269 | 18.117 | 20.099 | 16.282 | 1.00 | 32.69 | C |
| ATOM | 2063 | O   | ASP | A | 269 | 17.974 | 19.720 | 17.450 | 1.00 | 32.69 | O |
| ATOM | 2064 | CB  | ASP | A | 269 | 16.282 | 21.381 | 15.390 | 1.00 | 32.73 | C |
| ATOM | 2065 | CG  | ASP | A | 269 | 15.094 | 21.583 | 14.478 | 1.00 | 32.07 | C |
| ATOM | 2066 | OD1 | ASP | A | 269 | 15.023 | 21.039 | 13.367 | 1.00 | 33.96 | O |
| ATOM | 2067 | OD2 | ASP | A | 269 | 14.191 | 22.368 | 14.806 | 1.00 | 30.81 | O |
| ATOM | 2068 | N   | VAL | A | 270 | 19.234 | 20.667 | 15.854 | 1.00 | 32.97 | N |
| ATOM | 2069 | CA  | VAL | A | 270 | 20.376 | 20.839 | 16.715 | 1.00 | 32.97 | C |
| ATOM | 2070 | C   | VAL | A | 270 | 20.844 | 22.258 | 16.579 | 1.00 | 32.97 | C |
| ATOM | 2071 | O   | VAL | A | 270 | 21.130 | 22.716 | 15.488 | 1.00 | 33.40 | O |
| ATOM | 2072 | CB  | VAL | A | 270 | 21.485 | 19.896 | 16.323 | 1.00 | 32.94 | C |
| ATOM | 2073 | CG1 | VAL | A | 270 | 22.755 | 20.207 | 17.066 | 1.00 | 33.16 | C |
| ATOM | 2074 | CG2 | VAL | A | 270 | 21.069 | 18.519 | 16.646 | 1.00 | 33.14 | C |
| ATOM | 2075 | N   | LEU | A | 271 | 20.883 | 22.965 | 17.692 | 1.00 | 32.91 | N |
| ATOM | 2076 | CA  | LEU | A | 271 | 21.321 | 24.337 | 17.690 | 1.00 | 32.91 | C |
| ATOM | 2077 | C   | LEU | A | 271 | 22.770 | 24.395 | 18.129 | 1.00 | 32.95 | C |
| ATOM | 2078 | O   | LEU | A | 271 | 23.116 | 23.864 | 19.161 | 1.00 | 32.76 | O |
| ATOM | 2079 | CB  | LEU | A | 271 | 20.468 | 25.159 | 18.656 | 1.00 | 32.64 | C |
| ATOM | 2080 | CG  | LEU | A | 271 | 20.896 | 26.616 | 18.773 | 1.00 | 32.61 | C |
| ATOM | 2081 | CD1 | LEU | A | 271 | 20.989 | 27.276 | 17.405 | 1.00 | 32.23 | C |
| ATOM | 2082 | CD2 | LEU | A | 271 | 19.936 | 27.383 | 19.638 | 1.00 | 33.12 | C |
| ATOM | 2083 | N   | TYR | A | 272 | 23.633 | 25.006 | 17.333 | 1.00 | 33.19 | N |
| ATOM | 2084 | CA  | TYR | A | 272 | 24.989 | 25.215 | 17.791 | 1.00 | 33.39 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2085 | C   | TYR | A | 272 | 25.004 | 26.517 | 18.554 | 1.00 | 33.40 | C |
| ATOM | 2086 | O   | TYR | A | 272 | 24.834 | 27.560 | 17.950 | 1.00 | 33.42 | O |
| ATOM | 2087 | CB  | TYR | A | 272 | 25.991 | 25.297 | 16.633 | 1.00 | 33.28 | C |
| ATOM | 2088 | CG  | TYR | A | 272 | 27.376 | 25.802 | 17.039 | 1.00 | 32.43 | C |
| ATOM | 2089 | CD1 | TYR | A | 272 | 28.005 | 25.340 | 18.179 | 1.00 | 31.06 | C |
| ATOM | 2090 | CD2 | TYR | A | 272 | 28.047 | 26.746 | 16.267 | 1.00 | 32.28 | C |
| ATOM | 2091 | CE1 | TYR | A | 272 | 29.265 | 25.805 | 18.544 | 1.00 | 30.52 | C |
| ATOM | 2092 | CE2 | TYR | A | 272 | 29.300 | 27.213 | 16.622 | 1.00 | 30.88 | C |
| ATOM | 2093 | CZ  | TYR | A | 272 | 29.906 | 26.737 | 17.759 | 1.00 | 29.92 | C |
| ATOM | 2094 | OH  | TYR | A | 272 | 31.146 | 27.216 | 18.113 | 1.00 | 27.15 | O |
| ATOM | 2095 | N   | ILE | A | 273 | 25.178 | 26.438 | 19.872 | 1.00 | 33.69 | N |
| ATOM | 2096 | CA  | ILE | A | 273 | 25.350 | 27.609 | 20.734 | 1.00 | 33.97 | C |
| ATOM | 2097 | C   | ILE | A | 273 | 26.830 | 27.759 | 21.068 | 1.00 | 34.43 | C |
| ATOM | 2098 | O   | ILE | A | 273 | 27.332 | 27.113 | 21.998 | 1.00 | 34.76 | O |
| ATOM | 2099 | CB  | ILE | A | 273 | 24.595 | 27.436 | 22.032 | 1.00 | 33.75 | C |
| ATOM | 2100 | CG1 | ILE | A | 273 | 23.122 | 27.219 | 21.749 | 1.00 | 33.59 | C |
| ATOM | 2101 | CG2 | ILE | A | 273 | 24.779 | 28.654 | 22.896 | 1.00 | 33.60 | C |
| ATOM | 2102 | CD1 | ILE | A | 273 | 22.306 | 26.986 | 22.984 | 1.00 | 33.23 | C |
| ATOM | 2103 | N   | PRO | A | 274 | 27.519 | 28.630 | 20.345 | 1.00 | 34.61 | N |
| ATOM | 2104 | CA  | PRO | A | 274 | 28.965 | 28.780 | 20.485 | 1.00 | 34.92 | C |
| ATOM | 2105 | C   | PRO | A | 274 | 29.348 | 29.378 | 21.803 | 1.00 | 35.17 | C |
| ATOM | 2106 | O   | PRO | A | 274 | 28.639 | 30.252 | 22.300 | 1.00 | 35.16 | O |
| ATOM | 2107 | CB  | PRO | A | 274 | 29.333 | 29.771 | 19.382 | 1.00 | 35.09 | C |
| ATOM | 2108 | CG  | PRO | A | 274 | 28.113 | 29.929 | 18.551 | 1.00 | 35.02 | C |
| ATOM | 2109 | CD  | PRO | A | 274 | 26.957 | 29.584 | 19.388 | 1.00 | 34.69 | C |
| ATOM | 2110 | N   | MET | A | 275 | 30.476 | 28.927 | 22.339 | 1.00 | 35.69 | N |
| ATOM | 2111 | CA  | MET | A | 275 | 30.982 | 29.399 | 23.622 | 1.00 | 36.15 | C |
| ATOM | 2112 | C   | MET | A | 275 | 30.981 | 30.917 | 23.754 | 1.00 | 36.09 | C |
| ATOM | 2113 | O   | MET | A | 275 | 31.316 | 31.635 | 22.805 | 1.00 | 36.23 | O |
| ATOM | 2114 | CB  | MET | A | 275 | 32.400 | 28.928 | 23.805 | 1.00 | 36.23 | C |
| ATOM | 2115 | CG  | MET | A | 275 | 32.813 | 28.928 | 25.229 | 1.00 | 38.02 | C |
| ATOM | 2116 | SD  | MET | A | 275 | 34.361 | 28.108 | 25.442 | 1.00 | 42.07 | S |
| ATOM | 2117 | CE  | MET | A | 275 | 35.330 | 28.680 | 23.895 | 1.00 | 42.34 | C |
| ATOM | 2118 | N   | TYR | A | 276 | 30.611 | 31.401 | 24.935 | 1.00 | 35.76 | N |
| ATOM | 2119 | CA  | TYR | A | 276 | 30.574 | 32.833 | 25.191 | 1.00 | 35.62 | C |
| ATOM | 2120 | C   | TYR | A | 276 | 29.339 | 33.513 | 24.555 | 1.00 | 35.32 | C |
| ATOM | 2121 | O   | TYR | A | 276 | 29.048 | 34.653 | 24.866 | 1.00 | 35.15 | O |
| ATOM | 2122 | CB  | TYR | A | 276 | 31.921 | 33.510 | 24.804 | 1.00 | 35.75 | C |
| ATOM | 2123 | CG  | TYR | A | 276 | 33.049 | 33.221 | 25.822 | 1.00 | 35.70 | C |
| ATOM | 2124 | CD1 | TYR | A | 276 | 33.036 | 33.805 | 27.077 | 1.00 | 34.51 | C |
| ATOM | 2125 | CD2 | TYR | A | 276 | 34.103 | 32.356 | 25.521 | 1.00 | 35.30 | C |
| ATOM | 2126 | CE1 | TYR | A | 276 | 34.013 | 33.549 | 27.997 | 1.00 | 34.63 | C |
| ATOM | 2127 | CE2 | TYR | A | 276 | 35.100 | 32.085 | 26.446 | 1.00 | 35.01 | C |
| ATOM | 2128 | CZ  | TYR | A | 276 | 35.055 | 32.685 | 27.695 | 1.00 | 35.73 | C |
| ATOM | 2129 | OH  | TYR | A | 276 | 36.051 | 32.433 | 28.657 | 1.00 | 34.27 | O |
| ATOM | 2130 | N   | TRP | A | 277 | 28.573 | 32.838 | 23.708 | 1.00 | 35.19 | N |
| ATOM | 2131 | CA  | TRP | A | 277 | 27.353 | 33.491 | 23.224 | 1.00 | 35.20 | C |
| ATOM | 2132 | C   | TRP | A | 277 | 26.245 | 33.424 | 24.245 | 1.00 | 35.16 | C |
| ATOM | 2133 | O   | TRP | A | 277 | 25.947 | 32.369 | 24.797 | 1.00 | 35.08 | O |
| ATOM | 2134 | CB  | TRP | A | 277 | 26.806 | 32.880 | 21.944 | 1.00 | 35.27 | C |
| ATOM | 2135 | CG  | TRP | A | 277 | 27.538 | 33.286 | 20.784 | 1.00 | 34.70 | C |
| ATOM | 2136 | CD1 | TRP | A | 277 | 28.858 | 33.128 | 20.579 | 1.00 | 35.11 | C |
| ATOM | 2137 | CD2 | TRP | A | 277 | 27.020 | 33.945 | 19.639 | 1.00 | 35.27 | C |
| ATOM | 2138 | NE1 | TRP | A | 277 | 29.213 | 33.648 | 19.361 | 1.00 | 35.58 | N |
| ATOM | 2139 | CE2 | TRP | A | 277 | 28.094 | 34.156 | 18.761 | 1.00 | 34.89 | C |
| ATOM | 2140 | CE3 | TRP | A | 277 | 25.751 | 34.388 | 19.258 | 1.00 | 35.56 | C |
| ATOM | 2141 | CZ2 | TRP | A | 277 | 27.946 | 34.781 | 17.543 | 1.00 | 32.83 | C |
| ATOM | 2142 | CZ3 | TRP | A | 277 | 25.612 | 35.012 | 18.041 | 1.00 | 34.41 | C |
| ATOM | 2143 | CH2 | TRP | A | 277 | 26.704 | 35.199 | 17.201 | 1.00 | 33.11 | C |
| ATOM | 2144 | N   | TRP | A | 278 | 25.597 | 34.555 | 24.457 | 1.00 | 35.11 | N |
| ATOM | 2145 | CA  | TRP | A | 278 | 24.501 | 34.612 | 25.388 | 1.00 | 35.03 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2146 | C   | TRP | A | 278 | 23.334 | 33.859 | 24.838 | 1.00 | 35.14 | C |
| ATOM | 2147 | O   | TRP | A | 278 | 23.068 | 33.939 | 23.637 | 1.00 | 35.16 | O |
| ATOM | 2148 | CB  | TRP | A | 278 | 24.047 | 36.030 | 25.553 | 1.00 | 34.94 | C |
| ATOM | 2149 | CG  | TRP | A | 278 | 25.025 | 36.909 | 26.185 | 1.00 | 35.52 | C |
| ATOM | 2150 | CD1 | TRP | A | 278 | 26.030 | 37.597 | 25.584 | 1.00 | 35.77 | C |
| ATOM | 2151 | CD2 | TRP | A | 278 | 25.071 | 37.244 | 27.560 | 1.00 | 36.19 | C |
| ATOM | 2152 | NE1 | TRP | A | 278 | 26.713 | 38.336 | 26.518 | 1.00 | 36.09 | N |
| ATOM | 2153 | CE2 | TRP | A | 278 | 26.133 | 38.132 | 27.741 | 1.00 | 36.37 | C |
| ATOM | 2154 | CE3 | TRP | A | 278 | 24.312 | 36.876 | 28.668 | 1.00 | 36.48 | C |
| ATOM | 2155 | CZ2 | TRP | A | 278 | 26.463 | 38.637 | 28.976 | 1.00 | 37.12 | C |
| ATOM | 2156 | CZ3 | TRP | A | 278 | 24.636 | 37.375 | 29.877 | 1.00 | 36.37 | C |
| ATOM | 2157 | CH2 | TRP | A | 278 | 25.701 | 38.246 | 30.032 | 1.00 | 36.92 | C |
| ATOM | 2158 | N   | HIS | A | 279 | 22.620 | 33.133 | 25.692 | 1.00 | 35.10 | N |
| ATOM | 2159 | CA  | HIS | A | 279 | 21.400 | 32.516 | 25.218 | 1.00 | 35.20 | C |
| ATOM | 2160 | C   | HIS | A | 279 | 20.300 | 32.555 | 26.231 | 1.00 | 34.69 | C |
| ATOM | 2161 | O   | HIS | A | 279 | 20.540 | 32.348 | 27.414 | 1.00 | 34.75 | O |
| ATOM | 2162 | CB  | HIS | A | 279 | 21.624 | 31.079 | 24.764 | 1.00 | 35.73 | C |
| ATOM | 2163 | CG  | HIS | A | 279 | 22.403 | 30.236 | 25.727 | 1.00 | 37.15 | C |
| ATOM | 2164 | ND1 | HIS | A | 279 | 23.775 | 30.295 | 25.819 | 1.00 | 39.54 | N |
| ATOM | 2165 | CD2 | HIS | A | 279 | 22.010 | 29.283 | 26.609 | 1.00 | 38.10 | C |
| ATOM | 2166 | CE1 | HIS | A | 279 | 24.194 | 29.425 | 26.726 | 1.00 | 39.33 | C |
| ATOM | 2167 | NE2 | HIS | A | 279 | 23.143 | 28.797 | 27.221 | 1.00 | 37.68 | N |
| ATOM | 2168 | N   | HIS | A | 280 | 19.092 | 32.795 | 25.721 | 1.00 | 34.17 | N |
| ATOM | 2169 | CA  | HIS | A | 280 | 17.850 | 32.854 | 26.483 | 1.00 | 33.72 | C |
| ATOM | 2170 | C   | HIS | A | 280 | 16.960 | 31.779 | 25.901 | 1.00 | 33.50 | C |
| ATOM | 2171 | O   | HIS | A | 280 | 16.730 | 31.765 | 24.705 | 1.00 | 33.21 | O |
| ATOM | 2172 | CB  | HIS | A | 280 | 17.215 | 34.208 | 26.257 | 1.00 | 33.58 | C |
| ATOM | 2173 | CG  | HIS | A | 280 | 15.733 | 34.247 | 26.468 | 1.00 | 33.92 | C |
| ATOM | 2174 | ND1 | HIS | A | 280 | 15.151 | 34.997 | 27.464 | 1.00 | 33.67 | N |
| ATOM | 2175 | CD2 | HIS | A | 280 | 14.711 | 33.680 | 25.779 | 1.00 | 34.05 | C |
| ATOM | 2176 | CE1 | HIS | A | 280 | 13.838 | 34.874 | 27.395 | 1.00 | 33.47 | C |
| ATOM | 2177 | NE2 | HIS | A | 280 | 13.545 | 34.078 | 26.384 | 1.00 | 33.19 | N |
| ATOM | 2178 | N   | ILE | A | 281 | 16.425 | 30.892 | 26.723 | 1.00 | 33.62 | N |
| ATOM | 2179 | CA  | ILE | A | 281 | 15.699 | 29.755 | 26.176 | 1.00 | 33.56 | C |
| ATOM | 2180 | C   | ILE | A | 281 | 14.358 | 29.554 | 26.806 | 1.00 | 33.01 | C |
| ATOM | 2181 | O   | ILE | A | 281 | 14.242 | 29.475 | 28.012 | 1.00 | 32.55 | O |
| ATOM | 2182 | CB  | ILE | A | 281 | 16.554 | 28.501 | 26.300 | 1.00 | 33.91 | C |
| ATOM | 2183 | CG1 | ILE | A | 281 | 17.699 | 28.600 | 25.295 | 1.00 | 35.00 | C |
| ATOM | 2184 | CG2 | ILE | A | 281 | 15.752 | 27.277 | 25.988 | 1.00 | 34.05 | C |
| ATOM | 2185 | CD1 | ILE | A | 281 | 18.797 | 27.663 | 25.562 | 1.00 | 36.33 | C |
| ATOM | 2186 | N   | GLU | A | 282 | 13.343 | 29.445 | 25.960 | 1.00 | 33.12 | N |
| ATOM | 2187 | CA  | GLU | A | 282 | 11.977 | 29.342 | 26.441 | 1.00 | 33.13 | C |
| ATOM | 2188 | C   | GLU | A | 282 | 11.168 | 28.219 | 25.777 | 1.00 | 32.96 | C |
| ATOM | 2189 | O   | GLU | A | 282 | 11.252 | 27.988 | 24.577 | 1.00 | 32.94 | O |
| ATOM | 2190 | CB  | GLU | A | 282 | 11.290 | 30.707 | 26.327 | 1.00 | 33.06 | C |
| ATOM | 2191 | CG  | GLU | A | 282 | 11.065 | 31.250 | 24.925 | 1.00 | 33.43 | C |
| ATOM | 2192 | CD  | GLU | A | 282 | 10.529 | 32.682 | 24.951 | 1.00 | 33.96 | C |
| ATOM | 2193 | OE1 | GLU | A | 282 | 11.071 | 33.500 | 25.703 | 1.00 | 34.61 | O |
| ATOM | 2194 | OE2 | GLU | A | 282 | 9.563  | 33.009 | 24.236 | 1.00 | 35.15 | O |
| ATOM | 2195 | N   | SER | A | 283 | 10.431 | 27.497 | 26.607 | 1.00 | 32.96 | N |
| ATOM | 2196 | CA  | SER | A | 283 | 9.571  | 26.420 | 26.169 | 1.00 | 33.51 | C |
| ATOM | 2197 | C   | SER | A | 283 | 8.247  | 27.070 | 25.784 | 1.00 | 34.03 | C |
| ATOM | 2198 | O   | SER | A | 283 | 7.654  | 27.772 | 26.597 | 1.00 | 34.19 | O |
| ATOM | 2199 | CB  | SER | A | 283 | 9.375  | 25.408 | 27.303 | 1.00 | 33.43 | C |
| ATOM | 2200 | OG  | SER | A | 283 | 10.371 | 24.393 | 27.280 | 1.00 | 32.99 | O |
| ATOM | 2201 | N   | LEU | A | 284 | 7.769  | 26.828 | 24.565 | 1.00 | 34.36 | N |
| ATOM | 2202 | CA  | LEU | A | 284 | 6.610  | 27.553 | 24.081 | 1.00 | 34.81 | C |
| ATOM | 2203 | C   | LEU | A | 284 | 5.399  | 27.454 | 24.982 | 1.00 | 35.14 | C |
| ATOM | 2204 | O   | LEU | A | 284 | 5.128  | 26.425 | 25.599 | 1.00 | 35.08 | O |
| ATOM | 2205 | CB  | LEU | A | 284 | 6.226  | 27.131 | 22.670 | 1.00 | 35.02 | C |
| ATOM | 2206 | CG  | LEU | A | 284 | 7.302  | 27.255 | 21.596 | 1.00 | 35.52 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2207 | CD1 | LEU | A | 284 | 6.675  | 27.427 | 20.231 | 1.00 | 36.06 | C |
| ATOM | 2208 | CD2 | LEU | A | 284 | 8.197  | 28.404 | 21.862 | 1.00 | 36.37 | C |
| ATOM | 2209 | N   | LEU | A | 285 | 4.674  | 28.561 | 25.040 | 1.00 | 35.48 | N |
| ATOM | 2210 | CA  | LEU | A | 285 | 3.481  | 28.641 | 25.832 | 1.00 | 35.85 | C |
| ATOM | 2211 | C   | LEU | A | 285 | 2.509  | 27.670 | 25.255 | 1.00 | 36.11 | C |
| ATOM | 2212 | O   | LEU | A | 285 | 2.314  | 27.623 | 24.041 | 1.00 | 36.34 | O |
| ATOM | 2213 | CB  | LEU | A | 285 | 2.876  | 30.024 | 25.742 | 1.00 | 35.90 | C |
| ATOM | 2214 | CG  | LEU | A | 285 | 3.740  | 31.116 | 26.343 | 1.00 | 36.22 | C |
| ATOM | 2215 | CD1 | LEU | A | 285 | 3.271  | 32.449 | 25.821 | 1.00 | 36.13 | C |
| ATOM | 2216 | CD2 | LEU | A | 285 | 3.701  | 31.034 | 27.861 | 1.00 | 36.27 | C |
| ATOM | 2217 | N   | ASN | A | 286 | 1.909  | 26.879 | 26.128 | 1.00 | 36.14 | N |
| ATOM | 2218 | CA  | ASN | A | 286 | 0.890  | 25.958 | 25.703 | 1.00 | 36.04 | C |
| ATOM | 2219 | C   | ASN | A | 286 | 1.373  | 24.932 | 24.663 | 1.00 | 35.65 | C |
| ATOM | 2220 | O   | ASN | A | 286 | 0.593  | 24.471 | 23.833 | 1.00 | 35.84 | O |
| ATOM | 2221 | CB  | ASN | A | 286 | -0.283 | 26.792 | 25.191 | 1.00 | 36.33 | C |
| ATOM | 2222 | CG  | ASN | A | 286 | -0.805 | 27.766 | 26.254 | 1.00 | 36.97 | C |
| ATOM | 2223 | OD1 | ASN | A | 286 | -1.266 | 27.346 | 27.316 | 1.00 | 37.84 | O |
| ATOM | 2224 | ND2 | ASN | A | 286 | -0.716 | 29.067 | 25.977 | 1.00 | 37.29 | N |
| ATOM | 2225 | N   | GLY | A | 287 | 2.648  | 24.550 | 24.736 | 1.00 | 35.18 | N |
| ATOM | 2226 | CA  | GLY | A | 287 | 3.220  | 23.588 | 23.806 | 1.00 | 34.71 | C |
| ATOM | 2227 | C   | GLY | A | 287 | 3.556  | 22.252 | 24.428 | 1.00 | 34.44 | C |
| ATOM | 2228 | O   | GLY | A | 287 | 4.071  | 21.349 | 23.764 | 1.00 | 34.53 | O |
| ATOM | 2229 | N   | GLY | A | 288 | 3.255  | 22.106 | 25.706 | 1.00 | 34.18 | N |
| ATOM | 2230 | CA  | GLY | A | 288 | 3.521  | 20.858 | 26.371 | 1.00 | 34.22 | C |
| ATOM | 2231 | C   | GLY | A | 288 | 4.964  | 20.793 | 26.766 | 1.00 | 34.25 | C |
| ATOM | 2232 | O   | GLY | A | 288 | 5.727  | 21.719 | 26.523 | 1.00 | 34.28 | O |
| ATOM | 2233 | N   | ILE | A | 289 | 5.351  | 19.674 | 27.349 | 1.00 | 34.55 | N |
| ATOM | 2234 | CA  | ILE | A | 289 | 6.671  | 19.572 | 27.918 | 1.00 | 34.83 | C |
| ATOM | 2235 | C   | ILE | A | 289 | 7.702  | 19.529 | 26.837 | 1.00 | 34.87 | C |
| ATOM | 2236 | O   | ILE | A | 289 | 7.417  | 19.196 | 25.687 | 1.00 | 35.21 | O |
| ATOM | 2237 | CB  | ILE | A | 289 | 6.815  | 18.325 | 28.786 | 1.00 | 35.01 | C |
| ATOM | 2238 | CG1 | ILE | A | 289 | 7.018  | 17.091 | 27.924 | 1.00 | 35.30 | C |
| ATOM | 2239 | CG2 | ILE | A | 289 | 5.610  | 18.143 | 29.694 | 1.00 | 35.22 | C |
| ATOM | 2240 | CD1 | ILE | A | 289 | 7.654  | 15.972 | 28.698 | 1.00 | 35.70 | C |
| ATOM | 2241 | N   | THR | A | 290 | 8.921  | 19.853 | 27.219 | 1.00 | 34.80 | N |
| ATOM | 2242 | CA  | THR | A | 290 | 10.001 | 19.849 | 26.273 | 1.00 | 34.64 | C |
| ATOM | 2243 | C   | THR | A | 290 | 11.103 | 18.951 | 26.740 | 1.00 | 34.30 | C |
| ATOM | 2244 | O   | THR | A | 290 | 11.286 | 18.742 | 27.924 | 1.00 | 34.66 | O |
| ATOM | 2245 | CB  | THR | A | 290 | 10.522 | 21.258 | 26.094 | 1.00 | 34.75 | C |
| ATOM | 2246 | OG1 | THR | A | 290 | 10.747 | 21.863 | 27.375 | 1.00 | 34.33 | O |
| ATOM | 2247 | CG2 | THR | A | 290 | 9.455  | 22.105 | 25.458 | 1.00 | 34.98 | C |
| ATOM | 2248 | N   | ILE | A | 291 | 11.832 | 18.395 | 25.802 | 1.00 | 33.95 | N |
| ATOM | 2249 | CA  | ILE | A | 291 | 12.940 | 17.576 | 26.176 | 1.00 | 34.07 | C |
| ATOM | 2250 | C   | ILE | A | 291 | 14.091 | 17.963 | 25.310 | 1.00 | 33.73 | C |
| ATOM | 2251 | O   | ILE | A | 291 | 13.933 | 18.203 | 24.125 | 1.00 | 33.83 | O |
| ATOM | 2252 | CB  | ILE | A | 291 | 12.590 | 16.111 | 26.029 | 1.00 | 34.23 | C |
| ATOM | 2253 | CG1 | ILE | A | 291 | 11.439 | 15.793 | 26.967 | 1.00 | 34.84 | C |
| ATOM | 2254 | CG2 | ILE | A | 291 | 13.758 | 15.248 | 26.429 | 1.00 | 34.60 | C |
| ATOM | 2255 | CD1 | ILE | A | 291 | 11.021 | 14.384 | 26.946 | 1.00 | 35.22 | C |
| ATOM | 2256 | N   | THR | A | 292 | 15.254 | 18.062 | 25.913 | 1.00 | 33.47 | N |
| ATOM | 2257 | CA  | THR | A | 292 | 16.410 | 18.418 | 25.158 | 1.00 | 33.68 | C |
| ATOM | 2258 | C   | THR | A | 292 | 17.579 | 17.741 | 25.748 | 1.00 | 33.73 | C |
| ATOM | 2259 | O   | THR | A | 292 | 17.623 | 17.472 | 26.942 | 1.00 | 33.28 | O |
| ATOM | 2260 | CB  | THR | A | 292 | 16.725 | 19.921 | 25.265 | 1.00 | 33.93 | C |
| ATOM | 2261 | OG1 | THR | A | 292 | 15.590 | 20.725 | 24.921 | 1.00 | 33.80 | O |
| ATOM | 2262 | CG2 | THR | A | 292 | 17.774 | 20.293 | 24.245 | 1.00 | 34.05 | C |
| ATOM | 2263 | N   | VAL | A | 293 | 18.565 | 17.518 | 24.906 | 1.00 | 34.13 | N |
| ATOM | 2264 | CA  | VAL | A | 293 | 19.821 | 17.030 | 25.391 | 1.00 | 34.56 | C |
| ATOM | 2265 | C   | VAL | A | 293 | 20.935 | 17.867 | 24.813 | 1.00 | 34.79 | C |
| ATOM | 2266 | O   | VAL | A | 293 | 21.039 | 18.017 | 23.600 | 1.00 | 34.88 | O |
| ATOM | 2267 | CB  | VAL | A | 293 | 20.029 | 15.603 | 25.019 | 1.00 | 34.66 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2268 | CG1 | VAL | A | 293 | 21.473 | 15.238 | 25.222 | 1.00 | 35.24 | C |
| ATOM | 2269 | CG2 | VAL | A | 293 | 19.141 | 14.741 | 25.880 | 1.00 | 35.15 | C |
| ATOM | 2270 | N   | ASN | A | 294 | 21.768 | 18.433 | 25.681 | 1.00 | 34.82 | N |
| ATOM | 2271 | CA  | ASN | A | 294 | 22.890 | 19.187 | 25.174 | 1.00 | 34.61 | C |
| ATOM | 2272 | C   | ASN | A | 294 | 24.159 | 18.372 | 25.251 | 1.00 | 34.68 | C |
| ATOM | 2273 | O   | ASN | A | 294 | 24.220 | 17.350 | 25.934 | 1.00 | 34.28 | O |
| ATOM | 2274 | CB  | ASN | A | 294 | 23.036 | 20.571 | 25.829 | 1.00 | 34.77 | C |
| ATOM | 2275 | CG  | ASN | A | 294 | 23.676 | 20.533 | 27.197 | 1.00 | 33.90 | C |
| ATOM | 2276 | OD1 | ASN | A | 294 | 24.170 | 19.504 | 27.653 | 1.00 | 36.35 | O |
| ATOM | 2277 | ND2 | ASN | A | 294 | 23.658 | 21.670 | 27.868 | 1.00 | 30.46 | N |
| ATOM | 2278 | N   | PHE | A | 295 | 25.141 | 18.870 | 24.510 | 1.00 | 34.93 | N |
| ATOM | 2279 | CA  | PHE | A | 295 | 26.450 | 18.291 | 24.326 | 1.00 | 35.27 | C |
| ATOM | 2280 | C   | PHE | A | 295 | 27.467 | 19.411 | 24.552 | 1.00 | 35.69 | C |
| ATOM | 2281 | O   | PHE | A | 295 | 27.610 | 20.288 | 23.698 | 1.00 | 35.68 | O |
| ATOM | 2282 | CB  | PHE | A | 295 | 26.581 | 17.832 | 22.875 | 1.00 | 35.33 | C |
| ATOM | 2283 | CG  | PHE | A | 295 | 25.858 | 16.554 | 22.545 | 1.00 | 34.85 | C |
| ATOM | 2284 | CD1 | PHE | A | 295 | 24.492 | 16.549 | 22.332 | 1.00 | 35.36 | C |
| ATOM | 2285 | CD2 | PHE | A | 295 | 26.559 | 15.371 | 22.383 | 1.00 | 33.46 | C |
| ATOM | 2286 | CE1 | PHE | A | 295 | 23.841 | 15.378 | 21.996 | 1.00 | 35.19 | C |
| ATOM | 2287 | CE2 | PHE | A | 295 | 25.918 | 14.207 | 22.048 | 1.00 | 33.20 | C |
| ATOM | 2288 | CZ  | PHE | A | 295 | 24.566 | 14.202 | 21.853 | 1.00 | 34.09 | C |
| ATOM | 2289 | N   | TRP | A | 296 | 28.182 | 19.369 | 25.677 | 1.00 | 36.18 | N |
| ATOM | 2290 | CA  | TRP | A | 296 | 29.113 | 20.433 | 26.073 | 1.00 | 36.34 | C |
| ATOM | 2291 | C   | TRP | A | 296 | 30.534 | 19.963 | 25.938 | 1.00 | 36.50 | C |
| ATOM | 2292 | O   | TRP | A | 296 | 30.932 | 18.969 | 26.563 | 1.00 | 36.32 | O |
| ATOM | 2293 | CB  | TRP | A | 296 | 28.913 | 20.830 | 27.541 | 1.00 | 36.57 | C |
| ATOM | 2294 | CG  | TRP | A | 296 | 27.934 | 21.912 | 27.776 | 1.00 | 37.38 | C |
| ATOM | 2295 | CD1 | TRP | A | 296 | 26.997 | 22.361 | 26.909 | 1.00 | 38.36 | C |
| ATOM | 2296 | CD2 | TRP | A | 296 | 27.787 | 22.693 | 28.965 | 1.00 | 39.42 | C |
| ATOM | 2297 | NE1 | TRP | A | 296 | 26.275 | 23.384 | 27.473 | 1.00 | 38.20 | N |
| ATOM | 2298 | CE2 | TRP | A | 296 | 26.737 | 23.605 | 28.736 | 1.00 | 38.86 | C |
| ATOM | 2299 | CE3 | TRP | A | 296 | 28.450 | 22.730 | 30.204 | 1.00 | 40.74 | C |
| ATOM | 2300 | CZ2 | TRP | A | 296 | 26.327 | 24.529 | 29.682 | 1.00 | 41.03 | C |
| ATOM | 2301 | CZ3 | TRP | A | 296 | 28.037 | 23.665 | 31.160 | 1.00 | 40.86 | C |
| ATOM | 2302 | CH2 | TRP | A | 296 | 26.989 | 24.544 | 30.891 | 1.00 | 41.52 | C |
| ATOM | 2303 | N   | TYR | A | 297 | 31.303 | 20.719 | 25.162 | 1.00 | 36.60 | N |
| ATOM | 2304 | CA  | TYR | A | 297 | 32.703 | 20.442 | 24.923 | 1.00 | 36.79 | C |
| ATOM | 2305 | C   | TYR | A | 297 | 33.534 | 21.597 | 25.457 | 1.00 | 36.96 | C |
| ATOM | 2306 | O   | TYR | A | 297 | 33.117 | 22.734 | 25.363 | 1.00 | 36.32 | O |
| ATOM | 2307 | CB  | TYR | A | 297 | 32.923 | 20.291 | 23.423 | 1.00 | 36.93 | C |
| ATOM | 2308 | CG  | TYR | A | 297 | 32.280 | 19.054 | 22.868 | 1.00 | 37.30 | C |
| ATOM | 2309 | CD1 | TYR | A | 297 | 30.939 | 19.046 | 22.523 | 1.00 | 37.28 | C |
| ATOM | 2310 | CD2 | TYR | A | 297 | 33.008 | 17.880 | 22.716 | 1.00 | 36.72 | C |
| ATOM | 2311 | CE1 | TYR | A | 297 | 30.346 | 17.907 | 22.039 | 1.00 | 37.15 | C |
| ATOM | 2312 | CE2 | TYR | A | 297 | 32.423 | 16.747 | 22.226 | 1.00 | 35.89 | C |
| ATOM | 2313 | CZ  | TYR | A | 297 | 31.088 | 16.764 | 21.893 | 1.00 | 36.57 | C |
| ATOM | 2314 | OH  | TYR | A | 297 | 30.467 | 15.641 | 21.405 | 1.00 | 36.99 | O |
| ATOM | 2315 | N   | LYS | A | 298 | 34.696 | 21.303 | 26.039 | 1.00 | 37.93 | N |
| ATOM | 2316 | CA  | LYS | A | 298 | 35.615 | 22.347 | 26.495 | 1.00 | 38.45 | C |
| ATOM | 2317 | C   | LYS | A | 298 | 36.090 | 22.994 | 25.236 | 1.00 | 38.43 | C |
| ATOM | 2318 | O   | LYS | A | 298 | 36.245 | 22.320 | 24.229 | 1.00 | 38.55 | O |
| ATOM | 2319 | CB  | LYS | A | 298 | 36.835 | 21.782 | 27.233 | 1.00 | 38.67 | C |
| ATOM | 2320 | CG  | LYS | A | 298 | 36.634 | 21.550 | 28.737 | 1.00 | 40.58 | C |
| ATOM | 2321 | CD  | LYS | A | 298 | 37.928 | 21.093 | 29.484 | 1.00 | 42.63 | C |
| ATOM | 2322 | CE  | LYS | A | 298 | 37.631 | 20.622 | 30.951 | 1.00 | 44.00 | C |
| ATOM | 2323 | NZ  | LYS | A | 298 | 38.841 | 20.251 | 31.812 | 1.00 | 43.61 | N |
| ATOM | 2324 | N   | GLY | A | 299 | 36.347 | 24.286 | 25.277 | 1.00 | 38.82 | N |
| ATOM | 2325 | CA  | GLY | A | 299 | 36.768 | 24.976 | 24.080 | 1.00 | 39.19 | C |
| ATOM | 2326 | C   | GLY | A | 299 | 38.174 | 24.582 | 23.719 | 1.00 | 39.60 | C |
| ATOM | 2327 | O   | GLY | A | 299 | 38.859 | 23.930 | 24.502 | 1.00 | 39.93 | O |
| ATOM | 2328 | N   | ALA | A | 300 | 38.594 | 24.963 | 22.520 | 1.00 | 40.20 | N |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2329 | CA  | ALA | A | 300 | 39.963 | 24.751 | 22.072 | 1.00 | 40.70 | C |
| ATOM | 2330 | C   | ALA | A | 300 | 40.917 | 25.588 | 22.929 | 1.00 | 41.18 | C |
| ATOM | 2331 | O   | ALA | A | 300 | 40.483 | 26.417 | 23.722 | 1.00 | 41.25 | O |
| ATOM | 2332 | CB  | ALA | A | 300 | 40.085 | 25.143 | 20.616 | 1.00 | 40.64 | C |
| ATOM | 2333 | N   | PRO | A | 301 | 42.215 | 25.408 | 22.733 | 1.00 | 41.91 | N |
| ATOM | 2334 | CA  | PRO | A | 301 | 43.213 | 26.102 | 23.542 | 1.00 | 42.49 | C |
| ATOM | 2335 | C   | PRO | A | 301 | 43.448 | 27.541 | 23.128 | 1.00 | 43.14 | C |
| ATOM | 2336 | O   | PRO | A | 301 | 43.323 | 27.899 | 21.962 | 1.00 | 43.31 | O |
| ATOM | 2337 | CB  | PRO | A | 301 | 44.483 | 25.326 | 23.230 | 1.00 | 42.38 | C |
| ATOM | 2338 | CG  | PRO | A | 301 | 44.300 | 24.924 | 21.833 | 1.00 | 42.16 | C |
| ATOM | 2339 | CD  | PRO | A | 301 | 42.851 | 24.571 | 21.701 | 1.00 | 41.99 | C |
| ATOM | 2340 | N   | THR | A | 302 | 43.823 | 28.343 | 24.112 | 1.00 | 43.86 | N |
| ATOM | 2341 | CA  | THR | A | 302 | 44.199 | 29.726 | 23.915 | 1.00 | 44.26 | C |
| ATOM | 2342 | C   | THR | A | 302 | 45.588 | 29.732 | 23.318 | 1.00 | 44.56 | C |
| ATOM | 2343 | O   | THR | A | 302 | 46.524 | 29.337 | 24.011 | 1.00 | 44.82 | O |
| ATOM | 2344 | CB  | THR | A | 302 | 44.284 | 30.383 | 25.277 | 1.00 | 44.20 | C |
| ATOM | 2345 | OG1 | THR | A | 302 | 43.030 | 30.253 | 25.956 | 1.00 | 45.23 | O |
| ATOM | 2346 | CG2 | THR | A | 302 | 44.512 | 31.858 | 25.138 | 1.00 | 44.53 | C |
| ATOM | 2347 | N   | PRO | A | 303 | 45.770 | 30.229 | 22.091 | 1.00 | 44.72 | N |
| ATOM | 2348 | CA  | PRO | A | 303 | 47.083 | 30.128 | 21.438 | 1.00 | 44.51 | C |
| ATOM | 2349 | C   | PRO | A | 303 | 48.177 | 30.759 | 22.306 | 1.00 | 44.48 | C |
| ATOM | 2350 | O   | PRO | A | 303 | 47.835 | 31.522 | 23.221 | 1.00 | 44.02 | O |
| ATOM | 2351 | CB  | PRO | A | 303 | 46.897 | 30.929 | 20.145 | 1.00 | 44.55 | C |
| ATOM | 2352 | CG  | PRO | A | 303 | 45.426 | 30.929 | 19.904 | 1.00 | 44.28 | C |
| ATOM | 2353 | CD  | PRO | A | 303 | 44.834 | 31.040 | 21.288 | 1.00 | 44.71 | C |
| ATOM | 2354 | N   | GLU | A | 307 | 46.829 | 36.983 | 18.732 | 1.00 | 42.48 | N |
| ATOM | 2355 | CA  | GLU | A | 307 | 46.845 | 37.952 | 17.646 | 1.00 | 42.70 | C |
| ATOM | 2356 | C   | GLU | A | 307 | 45.812 | 39.039 | 17.801 | 1.00 | 42.57 | C |
| ATOM | 2357 | O   | GLU | A | 307 | 44.654 | 38.807 | 18.138 | 1.00 | 42.62 | O |
| ATOM | 2358 | CB  | GLU | A | 307 | 46.624 | 37.296 | 16.284 | 1.00 | 43.00 | C |
| ATOM | 2359 | CG  | GLU | A | 307 | 46.980 | 38.235 | 15.127 | 1.00 | 43.85 | C |
| ATOM | 2360 | CD  | GLU | A | 307 | 47.091 | 37.541 | 13.779 | 1.00 | 44.71 | C |
| ATOM | 2361 | OE1 | GLU | A | 307 | 46.618 | 36.385 | 13.643 | 1.00 | 45.10 | O |
| ATOM | 2362 | OE2 | GLU | A | 307 | 47.649 | 38.170 | 12.851 | 1.00 | 45.60 | O |
| ATOM | 2363 | N   | TYR | A | 308 | 46.249 | 40.243 | 17.503 | 1.00 | 42.66 | N |
| ATOM | 2364 | CA  | TYR | A | 308 | 45.384 | 41.379 | 17.577 | 1.00 | 42.64 | C |
| ATOM | 2365 | C   | TYR | A | 308 | 44.814 | 41.530 | 16.189 | 1.00 | 42.85 | C |
| ATOM | 2366 | O   | TYR | A | 308 | 45.413 | 41.066 | 15.203 | 1.00 | 43.43 | O |
| ATOM | 2367 | CB  | TYR | A | 308 | 46.184 | 42.565 | 18.034 | 1.00 | 42.47 | C |
| ATOM | 2368 | CG  | TYR | A | 308 | 46.744 | 42.281 | 19.399 | 1.00 | 43.35 | C |
| ATOM | 2369 | CD1 | TYR | A | 308 | 45.996 | 42.552 | 20.534 | 1.00 | 44.58 | C |
| ATOM | 2370 | CD2 | TYR | A | 308 | 47.986 | 41.681 | 19.559 | 1.00 | 43.97 | C |
| ATOM | 2371 | CE1 | TYR | A | 308 | 46.482 | 42.284 | 21.790 | 1.00 | 45.23 | C |
| ATOM | 2372 | CE2 | TYR | A | 308 | 48.483 | 41.401 | 20.818 | 1.00 | 44.79 | C |
| ATOM | 2373 | CZ  | TYR | A | 308 | 47.726 | 41.708 | 21.935 | 1.00 | 45.46 | C |
| ATOM | 2374 | OH  | TYR | A | 308 | 48.200 | 41.453 | 23.207 | 1.00 | 45.86 | O |
| ATOM | 2375 | N   | PRO | A | 309 | 43.631 | 42.119 | 16.111 | 1.00 | 42.47 | N |
| ATOM | 2376 | CA  | PRO | A | 309 | 42.930 | 42.648 | 17.285 | 1.00 | 42.08 | C |
| ATOM | 2377 | C   | PRO | A | 309 | 42.209 | 41.528 | 18.051 | 1.00 | 41.24 | C |
| ATOM | 2378 | O   | PRO | A | 309 | 41.774 | 40.578 | 17.408 | 1.00 | 40.92 | O |
| ATOM | 2379 | CB  | PRO | A | 309 | 41.910 | 43.583 | 16.652 | 1.00 | 42.39 | C |
| ATOM | 2380 | CG  | PRO | A | 309 | 41.574 | 42.895 | 15.337 | 1.00 | 42.16 | C |
| ATOM | 2381 | CD  | PRO | A | 309 | 42.843 | 42.260 | 14.874 | 1.00 | 42.28 | C |
| ATOM | 2382 | N   | LEU | A | 310 | 42.059 | 41.654 | 19.372 | 1.00 | 40.25 | N |
| ATOM | 2383 | CA  | LEU | A | 310 | 41.436 | 40.596 | 20.180 | 1.00 | 39.46 | C |
| ATOM | 2384 | C   | LEU | A | 310 | 39.971 | 40.434 | 19.884 | 1.00 | 38.93 | C |
| ATOM | 2385 | O   | LEU | A | 310 | 39.288 | 41.412 | 19.624 | 1.00 | 39.65 | O |
| ATOM | 2386 | CB  | LEU | A | 310 | 41.526 | 40.916 | 21.658 | 1.00 | 39.21 | C |
| ATOM | 2387 | CG  | LEU | A | 310 | 42.486 | 40.099 | 22.508 | 1.00 | 38.87 | C |
| ATOM | 2388 | CD1 | LEU | A | 310 | 43.727 | 39.738 | 21.750 | 1.00 | 38.58 | C |
| ATOM | 2389 | CD2 | LEU | A | 310 | 42.817 | 40.926 | 23.735 | 1.00 | 39.01 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2390 | N   | LYS | A | 311 | 39.462 | 39.217 | 19.957 | 1.00 | 37.90 | N |
| ATOM | 2391 | CA  | LYS | A | 311 | 38.036 | 39.029 | 19.731 | 1.00 | 37.53 | C |
| ATOM | 2392 | C   | LYS | A | 311 | 37.217 | 39.359 | 20.978 | 1.00 | 36.85 | C |
| ATOM | 2393 | O   | LYS | A | 311 | 37.705 | 39.272 | 22.092 | 1.00 | 36.85 | O |
| ATOM | 2394 | CB  | LYS | A | 311 | 37.746 | 37.609 | 19.274 | 1.00 | 37.54 | C |
| ATOM | 2395 | N   | ALA | A | 312 | 35.965 | 39.736 | 20.793 | 1.00 | 36.18 | N |
| ATOM | 2396 | CA  | ALA | A | 312 | 35.112 | 40.015 | 21.937 | 1.00 | 35.92 | C |
| ATOM | 2397 | C   | ALA | A | 312 | 35.232 | 38.994 | 23.058 | 1.00 | 35.88 | C |
| ATOM | 2398 | O   | ALA | A | 312 | 35.347 | 39.384 | 24.213 | 1.00 | 35.99 | O |
| ATOM | 2399 | CB  | ALA | A | 312 | 33.665 | 40.115 | 21.526 | 1.00 | 35.50 | C |
| ATOM | 2400 | N   | HIS | A | 313 | 35.221 | 37.700 | 22.739 | 1.00 | 35.71 | N |
| ATOM | 2401 | CA  | HIS | A | 313 | 35.136 | 36.709 | 23.797 | 1.00 | 35.52 | C |
| ATOM | 2402 | C   | HIS | A | 313 | 36.429 | 36.694 | 24.517 | 1.00 | 35.31 | C |
| ATOM | 2403 | O   | HIS | A | 313 | 36.489 | 36.278 | 25.667 | 1.00 | 35.53 | O |
| ATOM | 2404 | CB  | HIS | A | 313 | 34.768 | 35.291 | 23.313 | 1.00 | 35.89 | C |
| ATOM | 2405 | CG  | HIS | A | 313 | 35.844 | 34.613 | 22.535 | 1.00 | 36.41 | C |
| ATOM | 2406 | ND1 | HIS | A | 313 | 36.097 | 34.905 | 21.214 | 1.00 | 38.71 | N |
| ATOM | 2407 | CD2 | HIS | A | 313 | 36.741 | 33.665 | 22.889 | 1.00 | 37.90 | C |
| ATOM | 2408 | CE1 | HIS | A | 313 | 37.111 | 34.175 | 20.789 | 1.00 | 38.65 | C |
| ATOM | 2409 | NE2 | HIS | A | 313 | 37.524 | 33.416 | 21.788 | 1.00 | 38.60 | N |
| ATOM | 2410 | N   | GLN | A | 314 | 37.478 | 37.162 | 23.861 | 1.00 | 35.08 | N |
| ATOM | 2411 | CA  | GLN | A | 314 | 38.760 | 37.203 | 24.535 | 1.00 | 35.00 | C |
| ATOM | 2412 | C   | GLN | A | 314 | 38.706 | 38.301 | 25.576 | 1.00 | 34.62 | C |
| ATOM | 2413 | O   | GLN | A | 314 | 39.145 | 38.109 | 26.703 | 1.00 | 34.28 | O |
| ATOM | 2414 | CB  | GLN | A | 314 | 39.924 | 37.399 | 23.558 | 1.00 | 35.10 | C |
| ATOM | 2415 | CG  | GLN | A | 314 | 40.091 | 36.229 | 22.597 | 1.00 | 35.42 | C |
| ATOM | 2416 | CD  | GLN | A | 314 | 41.107 | 36.478 | 21.500 | 1.00 | 35.10 | C |
| ATOM | 2417 | OE1 | GLN | A | 314 | 40.938 | 37.377 | 20.671 | 1.00 | 35.86 | O |
| ATOM | 2418 | NE2 | GLN | A | 314 | 42.150 | 35.666 | 21.476 | 1.00 | 34.32 | N |
| ATOM | 2419 | N   | LYS | A | 315 | 38.173 | 39.454 | 25.197 | 1.00 | 34.70 | N |
| ATOM | 2420 | CA  | LYS | A | 315 | 38.009 | 40.539 | 26.152 | 1.00 | 35.01 | C |
| ATOM | 2421 | C   | LYS | A | 315 | 37.164 | 40.063 | 27.320 | 1.00 | 34.67 | C |
| ATOM | 2422 | O   | LYS | A | 315 | 37.485 | 40.325 | 28.467 | 1.00 | 34.81 | O |
| ATOM | 2423 | CB  | LYS | A | 315 | 37.395 | 41.766 | 25.501 | 1.00 | 35.19 | C |
| ATOM | 2424 | CG  | LYS | A | 315 | 38.344 | 42.447 | 24.563 | 1.00 | 35.85 | C |
| ATOM | 2425 | CD  | LYS | A | 315 | 37.703 | 43.636 | 23.931 | 1.00 | 37.25 | C |
| ATOM | 2426 | CE  | LYS | A | 315 | 38.657 | 44.348 | 23.001 | 1.00 | 39.28 | C |
| ATOM | 2427 | NZ  | LYS | A | 315 | 37.969 | 45.430 | 22.222 | 1.00 | 40.34 | N |
| ATOM | 2428 | N   | VAL | A | 316 | 36.117 | 39.314 | 27.040 | 1.00 | 34.30 | N |
| ATOM | 2429 | CA  | VAL | A | 316 | 35.321 | 38.787 | 28.118 | 1.00 | 34.31 | C |
| ATOM | 2430 | C   | VAL | A | 316 | 36.175 | 37.925 | 29.047 | 1.00 | 34.37 | C |
| ATOM | 2431 | O   | VAL | A | 316 | 36.071 | 38.023 | 30.273 | 1.00 | 34.57 | O |
| ATOM | 2432 | CB  | VAL | A | 316 | 34.138 | 37.992 | 27.606 | 1.00 | 34.39 | C |
| ATOM | 2433 | CG1 | VAL | A | 316 | 33.334 | 37.434 | 28.794 | 1.00 | 34.91 | C |
| ATOM | 2434 | CG2 | VAL | A | 316 | 33.258 | 38.873 | 26.719 | 1.00 | 33.60 | C |
| ATOM | 2435 | N   | ALA | A | 317 | 37.011 | 37.072 | 28.475 | 1.00 | 34.24 | N |
| ATOM | 2436 | CA  | ALA | A | 317 | 37.907 | 36.267 | 29.288 | 1.00 | 34.17 | C |
| ATOM | 2437 | C   | ALA | A | 317 | 38.744 | 37.160 | 30.166 | 1.00 | 34.10 | C |
| ATOM | 2438 | O   | ALA | A | 317 | 38.919 | 36.906 | 31.352 | 1.00 | 33.87 | O |
| ATOM | 2439 | CB  | ALA | A | 317 | 38.813 | 35.459 | 28.431 | 1.00 | 34.02 | C |
| ATOM | 2440 | N   | ILE | A | 318 | 39.274 | 38.216 | 29.574 | 1.00 | 34.29 | N |
| ATOM | 2441 | CA  | ILE | A | 318 | 40.178 | 39.062 | 30.322 | 1.00 | 34.26 | C |
| ATOM | 2442 | C   | ILE | A | 318 | 39.467 | 39.611 | 31.546 | 1.00 | 33.99 | C |
| ATOM | 2443 | O   | ILE | A | 318 | 39.993 | 39.556 | 32.661 | 1.00 | 33.96 | O |
| ATOM | 2444 | CB  | ILE | A | 318 | 40.755 | 40.171 | 29.447 | 1.00 | 33.98 | C |
| ATOM | 2445 | CG1 | ILE | A | 318 | 41.775 | 39.558 | 28.489 | 1.00 | 34.02 | C |
| ATOM | 2446 | CG2 | ILE | A | 318 | 41.429 | 41.188 | 30.323 | 1.00 | 33.92 | C |
| ATOM | 2447 | CD1 | ILE | A | 318 | 42.356 | 40.498 | 27.428 | 1.00 | 33.97 | C |
| ATOM | 2448 | N   | MET | A | 319 | 38.241 | 40.068 | 31.337 | 1.00 | 33.55 | N |
| ATOM | 2449 | CA  | MET | A | 319 | 37.499 | 40.741 | 32.383 | 1.00 | 33.41 | C |
| ATOM | 2450 | C   | MET | A | 319 | 37.196 | 39.772 | 33.496 | 1.00 | 33.38 | C |

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2451 | O   | MET | A | 319 | 37.238 | 40.101 | 34.669 | 1.00 | 33.32 | O |
| ATOM | 2452 | CB  | MET | A | 319 | 36.193 | 41.308 | 31.827 | 1.00 | 33.31 | C |
| ATOM | 2453 | CG  | MET | A | 319 | 36.361 | 42.521 | 30.951 | 1.00 | 32.96 | C |
| ATOM | 2454 | SD  | MET | A | 319 | 34.812 | 43.355 | 30.617 | 1.00 | 33.05 | S |
| ATOM | 2455 | CE  | MET | A | 319 | 34.119 | 42.299 | 29.410 | 1.00 | 33.43 | C |
| ATOM | 2456 | N   | ARG | A | 320 | 36.873 | 38.558 | 33.121 | 1.00 | 33.68 | N |
| ATOM | 2457 | CA  | ARG | A | 320 | 36.575 | 37.568 | 34.112 | 1.00 | 33.61 | C |
| ATOM | 2458 | C   | ARG | A | 320 | 37.796 | 37.392 | 34.996 | 1.00 | 33.82 | C |
| ATOM | 2459 | O   | ARG | A | 320 | 37.719 | 37.448 | 36.225 | 1.00 | 33.48 | O |
| ATOM | 2460 | CB  | ARG | A | 320 | 36.211 | 36.292 | 33.402 | 1.00 | 33.39 | C |
| ATOM | 2461 | CG  | ARG | A | 320 | 34.875 | 36.406 | 32.725 | 1.00 | 33.88 | C |
| ATOM | 2462 | CD  | ARG | A | 320 | 34.268 | 35.080 | 32.340 | 1.00 | 34.20 | C |
| ATOM | 2463 | NE  | ARG | A | 320 | 34.217 | 34.215 | 33.507 | 1.00 | 33.14 | N |
| ATOM | 2464 | CZ  | ARG | A | 320 | 33.159 | 34.103 | 34.260 | 1.00 | 33.15 | C |
| ATOM | 2465 | NH1 | ARG | A | 320 | 32.077 | 34.762 | 33.933 | 1.00 | 33.83 | N |
| ATOM | 2466 | NH2 | ARG | A | 320 | 33.170 | 33.338 | 35.331 | 1.00 | 34.46 | N |
| ATOM | 2467 | N   | ASN | A | 321 | 38.941 | 37.232 | 34.355 | 1.00 | 33.92 | N |
| ATOM | 2468 | CA  | ASN | A | 321 | 40.143 | 36.978 | 35.085 | 1.00 | 34.08 | C |
| ATOM | 2469 | C   | ASN | A | 321 | 40.486 | 38.141 | 36.018 | 1.00 | 34.26 | C |
| ATOM | 2470 | O   | ASN | A | 321 | 40.874 | 37.919 | 37.164 | 1.00 | 34.14 | O |
| ATOM | 2471 | CB  | ASN | A | 321 | 41.271 | 36.616 | 34.119 | 1.00 | 34.30 | C |
| ATOM | 2472 | CG  | ASN | A | 321 | 41.195 | 35.161 | 33.663 | 1.00 | 34.44 | C |
| ATOM | 2473 | OD1 | ASN | A | 321 | 40.829 | 34.273 | 34.434 | 1.00 | 34.16 | O |
| ATOM | 2474 | ND2 | ASN | A | 321 | 41.522 | 34.918 | 32.402 | 1.00 | 35.05 | N |
| ATOM | 2475 | N   | ILE | A | 322 | 40.318 | 39.379 | 35.569 | 1.00 | 34.24 | N |
| ATOM | 2476 | CA  | ILE | A | 322 | 40.634 | 40.488 | 36.448 | 1.00 | 34.25 | C |
| ATOM | 2477 | C   | ILE | A | 322 | 39.781 | 40.408 | 37.701 | 1.00 | 33.85 | C |
| ATOM | 2478 | O   | ILE | A | 322 | 40.250 | 40.711 | 38.789 | 1.00 | 34.16 | O |
| ATOM | 2479 | CB  | ILE | A | 322 | 40.412 | 41.837 | 35.760 | 1.00 | 34.70 | C |
| ATOM | 2480 | CG1 | ILE | A | 322 | 41.338 | 41.993 | 34.558 | 1.00 | 35.34 | C |
| ATOM | 2481 | CG2 | ILE | A | 322 | 40.651 | 43.007 | 36.748 | 1.00 | 35.37 | C |
| ATOM | 2482 | CD1 | ILE | A | 322 | 42.778 | 41.928 | 34.895 | 1.00 | 36.17 | C |
| ATOM | 2483 | N   | GLU | A | 323 | 38.525 | 40.013 | 37.558 | 1.00 | 33.42 | N |
| ATOM | 2484 | CA  | GLU | A | 323 | 37.636 | 39.935 | 38.704 | 1.00 | 32.97 | C |
| ATOM | 2485 | C   | GLU | A | 323 | 38.085 | 38.842 | 39.652 | 1.00 | 33.11 | C |
| ATOM | 2486 | O   | GLU | A | 323 | 38.067 | 39.001 | 40.864 | 1.00 | 32.66 | O |
| ATOM | 2487 | CB  | GLU | A | 323 | 36.199 | 39.673 | 38.256 | 1.00 | 32.73 | C |
| ATOM | 2488 | CG  | GLU | A | 323 | 35.543 | 40.907 | 37.672 | 1.00 | 33.02 | C |
| ATOM | 2489 | CD  | GLU | A | 323 | 34.166 | 40.693 | 37.057 | 1.00 | 32.91 | C |
| ATOM | 2490 | OE1 | GLU | A | 323 | 33.193 | 40.309 | 37.740 | 1.00 | 31.94 | O |
| ATOM | 2491 | OE2 | GLU | A | 323 | 34.048 | 40.961 | 35.856 | 1.00 | 33.81 | O |
| ATOM | 2492 | N   | LYS | A | 324 | 38.497 | 37.720 | 39.088 | 1.00 | 33.56 | N |
| ATOM | 2493 | CA  | LYS | A | 324 | 38.882 | 36.588 | 39.895 | 1.00 | 33.72 | C |
| ATOM | 2494 | C   | LYS | A | 324 | 40.138 | 36.937 | 40.670 | 1.00 | 34.09 | C |
| ATOM | 2495 | O   | LYS | A | 324 | 40.228 | 36.664 | 41.859 | 1.00 | 34.15 | O |
| ATOM | 2496 | CB  | LYS | A | 324 | 39.119 | 35.368 | 39.012 | 1.00 | 33.73 | C |
| ATOM | 2497 | CG  | LYS | A | 324 | 37.877 | 34.766 | 38.353 | 1.00 | 33.83 | C |
| ATOM | 2498 | CD  | LYS | A | 324 | 38.355 | 33.673 | 37.440 | 1.00 | 33.70 | C |
| ATOM | 2499 | CE  | LYS | A | 324 | 37.294 | 32.883 | 36.723 | 1.00 | 33.57 | C |
| ATOM | 2500 | NZ  | LYS | A | 324 | 37.993 | 31.761 | 35.984 | 1.00 | 32.76 | N |
| ATOM | 2501 | N   | MET | A | 325 | 41.098 | 37.558 | 39.995 | 1.00 | 34.73 | N |
| ATOM | 2502 | CA  | MET | A | 325 | 42.380 | 37.915 | 40.609 | 1.00 | 35.32 | C |
| ATOM | 2503 | C   | MET | A | 325 | 42.248 | 38.883 | 41.766 | 1.00 | 35.06 | C |
| ATOM | 2504 | O   | MET | A | 325 | 42.888 | 38.729 | 42.808 | 1.00 | 34.50 | O |
| ATOM | 2505 | CB  | MET | A | 325 | 43.328 | 38.501 | 39.563 | 1.00 | 35.57 | C |
| ATOM | 2506 | CG  | MET | A | 325 | 43.962 | 37.419 | 38.724 | 1.00 | 36.96 | C |
| ATOM | 2507 | SD  | MET | A | 325 | 44.984 | 37.973 | 37.360 | 1.00 | 40.43 | S |
| ATOM | 2508 | CE  | MET | A | 325 | 45.710 | 39.363 | 38.037 | 1.00 | 41.05 | C |
| ATOM | 2509 | N   | LEU | A | 326 | 41.427 | 39.891 | 41.555 | 1.00 | 35.32 | N |
| ATOM | 2510 | CA  | LEU | A | 326 | 41.178 | 40.895 | 42.570 | 1.00 | 35.83 | C |
| ATOM | 2511 | C   | LEU | A | 326 | 40.556 | 40.230 | 43.770 | 1.00 | 35.60 | C |



|      |      |     |           |        |        |        |      |       |   |
|------|------|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 2512 | O   | LEU A 326 | 40.914 | 40.507 | 44.910 | 1.00 | 35.34 | O |
| ATOM | 2513 | CB  | LEU A 326 | 40.216 | 41.929 | 42.026 | 1.00 | 36.07 | C |
| ATOM | 2514 | CG  | LEU A 326 | 40.721 | 43.321 | 41.689 | 1.00 | 37.48 | C |
| ATOM | 2515 | CD1 | LEU A 326 | 42.221 | 43.442 | 41.537 | 1.00 | 38.59 | C |
| ATOM | 2516 | CD2 | LEU A 326 | 40.049 | 43.692 | 40.413 | 1.00 | 38.65 | C |
| ATOM | 2517 | N   | GLY A 327 | 39.613 | 39.341 | 43.493 | 1.00 | 35.59 | N |
| ATOM | 2518 | CA  | GLY A 327 | 38.947 | 38.604 | 44.538 | 1.00 | 35.54 | C |
| ATOM | 2519 | C   | GLY A 327 | 39.983 | 37.998 | 45.443 | 1.00 | 35.62 | C |
| ATOM | 2520 | O   | GLY A 327 | 40.023 | 38.258 | 46.641 | 1.00 | 35.52 | O |
| ATOM | 2521 | N   | GLU A 328 | 40.863 | 37.209 | 44.851 | 1.00 | 35.84 | N |
| ATOM | 2522 | CA  | GLU A 328 | 41.831 | 36.486 | 45.632 | 1.00 | 35.91 | C |
| ATOM | 2523 | C   | GLU A 328 | 42.783 | 37.424 | 46.298 | 1.00 | 35.44 | C |
| ATOM | 2524 | O   | GLU A 328 | 43.086 | 37.272 | 47.465 | 1.00 | 35.60 | O |
| ATOM | 2525 | CB  | GLU A 328 | 42.584 | 35.513 | 44.750 | 1.00 | 36.21 | C |
| ATOM | 2526 | CG  | GLU A 328 | 41.675 | 34.419 | 44.226 | 1.00 | 38.20 | C |
| ATOM | 2527 | CD  | GLU A 328 | 41.854 | 33.088 | 44.941 | 1.00 | 41.33 | C |
| ATOM | 2528 | OE1 | GLU A 328 | 42.244 | 33.084 | 46.138 | 1.00 | 42.40 | O |
| ATOM | 2529 | OE2 | GLU A 328 | 41.608 | 32.034 | 44.292 | 1.00 | 43.59 | O |
| ATOM | 2530 | N   | ALA A 329 | 43.220 | 38.435 | 45.577 | 1.00 | 35.11 | N |
| ATOM | 2531 | CA  | ALA A 329 | 44.259 | 39.282 | 46.110 | 1.00 | 34.85 | C |
| ATOM | 2532 | C   | ALA A 329 | 43.790 | 40.103 | 47.296 | 1.00 | 34.75 | C |
| ATOM | 2533 | O   | ALA A 329 | 44.533 | 40.282 | 48.258 | 1.00 | 34.53 | O |
| ATOM | 2534 | CB  | ALA A 329 | 44.778 | 40.163 | 45.046 | 1.00 | 34.85 | C |
| ATOM | 2535 | N   | LEU A 330 | 42.567 | 40.613 | 47.214 | 1.00 | 34.62 | N |
| ATOM | 2536 | CA  | LEU A 330 | 41.996 | 41.399 | 48.291 | 1.00 | 34.55 | C |
| ATOM | 2537 | C   | LEU A 330 | 41.478 | 40.555 | 49.448 | 1.00 | 34.90 | C |
| ATOM | 2538 | O   | LEU A 330 | 41.234 | 41.072 | 50.532 | 1.00 | 35.33 | O |
| ATOM | 2539 | CB  | LEU A 330 | 40.851 | 42.245 | 47.766 | 1.00 | 34.31 | C |
| ATOM | 2540 | CG  | LEU A 330 | 41.202 | 43.322 | 46.743 | 1.00 | 34.06 | C |
| ATOM | 2541 | CD1 | LEU A 330 | 39.942 | 43.965 | 46.258 | 1.00 | 34.23 | C |
| ATOM | 2542 | CD2 | LEU A 330 | 42.078 | 44.382 | 47.285 | 1.00 | 34.05 | C |
| ATOM | 2543 | N   | GLY A 331 | 41.295 | 39.262 | 49.232 | 1.00 | 35.23 | N |
| ATOM | 2544 | CA  | GLY A 331 | 40.794 | 38.401 | 50.285 | 1.00 | 35.49 | C |
| ATOM | 2545 | C   | GLY A 331 | 39.306 | 38.471 | 50.584 | 1.00 | 35.66 | C |
| ATOM | 2546 | O   | GLY A 331 | 38.849 | 37.859 | 51.544 | 1.00 | 35.61 | O |
| ATOM | 2547 | N   | ASN A 332 | 38.547 | 39.213 | 49.790 | 1.00 | 36.04 | N |
| ATOM | 2548 | CA  | ASN A 332 | 37.113 | 39.295 | 49.992 | 1.00 | 36.44 | C |
| ATOM | 2549 | C   | ASN A 332 | 36.483 | 39.791 | 48.732 | 1.00 | 36.55 | C |
| ATOM | 2550 | O   | ASN A 332 | 36.647 | 40.951 | 48.381 | 1.00 | 37.01 | O |
| ATOM | 2551 | CB  | ASN A 332 | 36.775 | 40.275 | 51.094 | 1.00 | 36.54 | C |
| ATOM | 2552 | CG  | ASN A 332 | 35.311 | 40.260 | 51.440 | 1.00 | 37.47 | C |
| ATOM | 2553 | OD1 | ASN A 332 | 34.519 | 39.541 | 50.828 | 1.00 | 37.83 | O |
| ATOM | 2554 | ND2 | ASN A 332 | 34.938 | 41.043 | 52.444 | 1.00 | 39.90 | N |
| ATOM | 2555 | N   | PRO A 333 | 35.699 | 38.957 | 48.078 | 1.00 | 36.46 | N |
| ATOM | 2556 | CA  | PRO A 333 | 35.178 | 39.338 | 46.775 | 1.00 | 36.43 | C |
| ATOM | 2557 | C   | PRO A 333 | 34.368 | 40.590 | 46.908 | 1.00 | 36.32 | C |
| ATOM | 2558 | O   | PRO A 333 | 34.318 | 41.384 | 45.988 | 1.00 | 36.36 | O |
| ATOM | 2559 | CB  | PRO A 333 | 34.278 | 38.170 | 46.366 | 1.00 | 36.50 | C |
| ATOM | 2560 | CG  | PRO A 333 | 34.247 | 37.229 | 47.489 | 1.00 | 36.58 | C |
| ATOM | 2561 | CD  | PRO A 333 | 35.180 | 37.668 | 48.548 | 1.00 | 36.54 | C |
| ATOM | 2562 | N   | GLN A 334 | 33.743 | 40.800 | 48.047 | 1.00 | 36.44 | N |
| ATOM | 2563 | CA  | GLN A 334 | 32.906 | 41.969 | 48.130 | 1.00 | 36.85 | C |
| ATOM | 2564 | C   | GLN A 334 | 33.748 | 43.222 | 48.057 | 1.00 | 36.57 | C |
| ATOM | 2565 | O   | GLN A 334 | 33.218 | 44.304 | 47.868 | 1.00 | 36.98 | O |
| ATOM | 2566 | CB  | GLN A 334 | 31.987 | 41.940 | 49.348 | 1.00 | 37.31 | C |
| ATOM | 2567 | CG  | GLN A 334 | 30.685 | 41.151 | 49.026 | 1.00 | 38.95 | C |
| ATOM | 2568 | CD  | GLN A 334 | 29.669 | 41.097 | 50.171 | 1.00 | 40.33 | C |
| ATOM | 2569 | OE1 | GLN A 334 | 29.751 | 41.872 | 51.137 | 1.00 | 41.70 | O |
| ATOM | 2570 | NE2 | GLN A 334 | 28.712 | 40.178 | 50.061 | 1.00 | 39.80 | N |
| ATOM | 2571 | N   | GLU A 335 | 35.064 | 43.088 | 48.159 | 1.00 | 35.99 | N |
| ATOM | 2572 | CA  | GLU A 335 | 35.914 | 44.261 | 48.067 | 1.00 | 35.53 | C |



|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2573 | C   | GLU | A | 335 | 36.229 | 44.610 | 46.621 | 1.00 | 34.53 | C |
| ATOM | 2574 | O   | GLU | A | 335 | 36.715 | 45.689 | 46.338 | 1.00 | 34.20 | O |
| ATOM | 2575 | CB  | GLU | A | 335 | 37.201 | 44.083 | 48.894 | 1.00 | 35.99 | C |
| ATOM | 2576 | CG  | GLU | A | 335 | 37.054 | 44.507 | 50.354 | 1.00 | 37.38 | C |
| ATOM | 2577 | CD  | GLU | A | 335 | 38.382 | 44.592 | 51.076 | 1.00 | 40.16 | C |
| ATOM | 2578 | OE1 | GLU | A | 335 | 39.271 | 45.318 | 50.570 | 1.00 | 42.04 | O |
| ATOM | 2579 | OE2 | GLU | A | 335 | 38.535 | 43.952 | 52.153 | 1.00 | 41.52 | O |
| ATOM | 2580 | N   | VAL | A | 336 | 35.922 | 43.701 | 45.706 | 1.00 | 33.97 | N |
| ATOM | 2581 | CA  | VAL | A | 336 | 36.165 | 43.901 | 44.276 | 1.00 | 33.49 | C |
| ATOM | 2582 | C   | VAL | A | 336 | 35.537 | 45.159 | 43.670 | 1.00 | 33.00 | C |
| ATOM | 2583 | O   | VAL | A | 336 | 36.194 | 45.904 | 42.946 | 1.00 | 33.01 | O |
| ATOM | 2584 | CB  | VAL | A | 336 | 35.696 | 42.678 | 43.473 | 1.00 | 33.36 | C |
| ATOM | 2585 | CG1 | VAL | A | 336 | 35.726 | 42.951 | 41.992 | 1.00 | 34.05 | C |
| ATOM | 2586 | CG2 | VAL | A | 336 | 36.582 | 41.509 | 43.755 | 1.00 | 33.01 | C |
| ATOM | 2587 | N   | GLY | A | 337 | 34.270 | 45.406 | 43.926 | 1.00 | 32.41 | N |
| ATOM | 2588 | CA  | GLY | A | 337 | 33.675 | 46.592 | 43.351 | 1.00 | 32.21 | C |
| ATOM | 2589 | C   | GLY | A | 337 | 34.332 | 47.903 | 43.724 | 1.00 | 31.72 | C |
| ATOM | 2590 | O   | GLY | A | 337 | 34.682 | 48.711 | 42.859 | 1.00 | 31.40 | O |
| ATOM | 2591 | N   | PRO | A | 338 | 34.433 | 48.163 | 45.013 | 1.00 | 31.50 | N |
| ATOM | 2592 | CA  | PRO | A | 338 | 35.025 | 49.415 | 45.470 | 1.00 | 31.47 | C |
| ATOM | 2593 | C   | PRO | A | 338 | 36.387 | 49.648 | 44.846 | 1.00 | 31.60 | C |
| ATOM | 2594 | O   | PRO | A | 338 | 36.655 | 50.756 | 44.386 | 1.00 | 31.51 | O |
| ATOM | 2595 | CB  | PRO | A | 338 | 35.065 | 49.230 | 46.977 | 1.00 | 31.27 | C |
| ATOM | 2596 | CG  | PRO | A | 338 | 33.883 | 48.376 | 47.218 | 1.00 | 31.08 | C |
| ATOM | 2597 | CD  | PRO | A | 338 | 33.933 | 47.359 | 46.137 | 1.00 | 31.28 | C |
| ATOM | 2598 | N   | LEU | A | 339 | 37.219 | 48.620 | 44.765 | 1.00 | 31.80 | N |
| ATOM | 2599 | CA  | LEU | A | 339 | 38.531 | 48.825 | 44.182 | 1.00 | 32.25 | C |
| ATOM | 2600 | C   | LEU | A | 339 | 38.431 | 49.269 | 42.740 | 1.00 | 32.12 | C |
| ATOM | 2601 | O   | LEU | A | 339 | 39.130 | 50.188 | 42.320 | 1.00 | 32.25 | O |
| ATOM | 2602 | CB  | LEU | A | 339 | 39.395 | 47.581 | 44.278 | 1.00 | 32.49 | C |
| ATOM | 2603 | CG  | LEU | A | 339 | 40.853 | 47.920 | 43.962 | 1.00 | 33.78 | C |
| ATOM | 2604 | CD1 | LEU | A | 339 | 41.793 | 47.121 | 44.797 | 1.00 | 34.64 | C |
| ATOM | 2605 | CD2 | LEU | A | 339 | 41.146 | 47.681 | 42.516 | 1.00 | 34.50 | C |
| ATOM | 2606 | N   | LEU | A | 340 | 37.567 | 48.607 | 41.978 | 1.00 | 32.12 | N |
| ATOM | 2607 | CA  | LEU | A | 340 | 37.385 | 48.963 | 40.584 | 1.00 | 31.85 | C |
| ATOM | 2608 | C   | LEU | A | 340 | 36.854 | 50.376 | 40.483 | 1.00 | 31.56 | C |
| ATOM | 2609 | O   | LEU | A | 340 | 37.342 | 51.169 | 39.701 | 1.00 | 31.42 | O |
| ATOM | 2610 | CB  | LEU | A | 340 | 36.468 | 47.975 | 39.888 | 1.00 | 31.90 | C |
| ATOM | 2611 | CG  | LEU | A | 340 | 37.089 | 46.598 | 39.669 | 1.00 | 32.44 | C |
| ATOM | 2612 | CD1 | LEU | A | 340 | 36.028 | 45.636 | 39.132 | 1.00 | 33.11 | C |
| ATOM | 2613 | CD2 | LEU | A | 340 | 38.281 | 46.660 | 38.728 | 1.00 | 31.95 | C |
| ATOM | 2614 | N   | ASN | A | 341 | 35.865 | 50.717 | 41.282 | 1.00 | 31.61 | N |
| ATOM | 2615 | CA  | ASN | A | 341 | 35.384 | 52.083 | 41.231 | 1.00 | 31.82 | C |
| ATOM | 2616 | C   | ASN | A | 341 | 36.484 | 53.109 | 41.525 | 1.00 | 31.45 | C |
| ATOM | 2617 | O   | ASN | A | 341 | 36.600 | 54.119 | 40.845 | 1.00 | 30.80 | O |
| ATOM | 2618 | CB  | ASN | A | 341 | 34.212 | 52.260 | 42.177 | 1.00 | 31.97 | C |
| ATOM | 2619 | CG  | ASN | A | 341 | 32.901 | 51.883 | 41.532 | 1.00 | 32.77 | C |
| ATOM | 2620 | OD1 | ASN | A | 341 | 32.426 | 52.568 | 40.614 | 1.00 | 34.75 | O |
| ATOM | 2621 | ND2 | ASN | A | 341 | 32.310 | 50.789 | 41.992 | 1.00 | 31.86 | N |
| ATOM | 2622 | N   | THR | A | 342 | 37.301 | 52.835 | 42.530 | 1.00 | 31.40 | N |
| ATOM | 2623 | CA  | THR | A | 342 | 38.380 | 53.739 | 42.880 | 1.00 | 31.27 | C |
| ATOM | 2624 | C   | THR | A | 342 | 39.317 | 53.842 | 41.707 | 1.00 | 31.14 | C |
| ATOM | 2625 | O   | THR | A | 342 | 39.837 | 54.908 | 41.402 | 1.00 | 30.66 | O |
| ATOM | 2626 | CB  | THR | A | 342 | 39.146 | 53.217 | 44.097 | 1.00 | 31.43 | C |
| ATOM | 2627 | OG1 | THR | A | 342 | 38.448 | 53.565 | 45.299 | 1.00 | 30.95 | O |
| ATOM | 2628 | CG2 | THR | A | 342 | 40.500 | 53.913 | 44.228 | 1.00 | 31.17 | C |
| ATOM | 2629 | N   | MET | A | 343 | 39.549 | 52.714 | 41.059 | 1.00 | 31.29 | N |
| ATOM | 2630 | CA  | MET | A | 343 | 40.406 | 52.703 | 39.898 | 1.00 | 31.59 | C |
| ATOM | 2631 | C   | MET | A | 343 | 39.970 | 53.639 | 38.785 | 1.00 | 31.49 | C |
| ATOM | 2632 | O   | MET | A | 343 | 40.804 | 54.361 | 38.255 | 1.00 | 31.46 | O |
| ATOM | 2633 | CB  | MET | A | 343 | 40.516 | 51.310 | 39.314 | 1.00 | 31.79 | C |

|        |      |     |     |       |     |        |        |        |      |       |    |
|--------|------|-----|-----|-------|-----|--------|--------|--------|------|-------|----|
| ATOM   | 2634 | CG  | MET | A     | 343 | 41.831 | 50.662 | 39.629 | 1.00 | 32.65 | C  |
| ATOM   | 2635 | SD  | MET | A     | 343 | 42.271 | 49.379 | 38.468 | 1.00 | 33.09 | S  |
| ATOM   | 2636 | CE  | MET | A     | 343 | 41.116 | 48.304 | 38.916 | 1.00 | 34.22 | C  |
| ATOM   | 2637 | N   | ILE | A     | 344 | 38.690 | 53.641 | 38.418 | 1.00 | 31.31 | N  |
| ATOM   | 2638 | CA  | ILE | A     | 344 | 38.293 | 54.432 | 37.265 | 1.00 | 31.42 | C  |
| ATOM   | 2639 | C   | ILE | A     | 344 | 37.708 | 55.787 | 37.533 | 1.00 | 31.14 | C  |
| ATOM   | 2640 | O   | ILE | A     | 344 | 37.752 | 56.630 | 36.640 | 1.00 | 31.01 | O  |
| ATOM   | 2641 | CB  | ILE | A     | 344 | 37.272 | 53.708 | 36.362 | 1.00 | 31.86 | C  |
| ATOM   | 2642 | CG1 | ILE | A     | 344 | 35.870 | 53.866 | 36.928 | 1.00 | 33.16 | C  |
| ATOM   | 2643 | CG2 | ILE | A     | 344 | 37.633 | 52.229 | 36.118 | 1.00 | 32.09 | C  |
| ATOM   | 2644 | CD1 | ILE | A     | 344 | 34.876 | 53.232 | 36.072 | 1.00 | 35.18 | C  |
| ATOM   | 2645 | N   | LYS | A     | 345 | 37.131 | 56.050 | 38.698 | 1.00 | 30.88 | N  |
| ATOM   | 2646 | CA  | LYS | A     | 345 | 36.455 | 57.334 | 38.758 | 1.00 | 30.94 | C  |
| ATOM   | 2647 | C   | LYS | A     | 345 | 37.412 | 58.468 | 38.853 | 1.00 | 30.72 | C  |
| ATOM   | 2648 | O   | LYS | A     | 345 | 38.250 | 58.558 | 39.743 | 1.00 | 30.61 | O  |
| ATOM   | 2649 | CB  | LYS | A     | 345 | 35.315 | 57.475 | 39.765 | 1.00 | 31.14 | C  |
| ATOM   | 2650 | CG  | LYS | A     | 345 | 35.361 | 56.680 | 40.977 | 1.00 | 32.16 | C  |
| ATOM   | 2651 | CD  | LYS | A     | 345 | 33.970 | 56.273 | 41.340 | 1.00 | 33.62 | C  |
| ATOM   | 2652 | CE  | LYS | A     | 345 | 33.514 | 56.873 | 42.665 | 1.00 | 34.71 | C  |
| ATOM   | 2653 | NZ  | LYS | A     | 345 | 34.302 | 56.317 | 43.840 | 1.00 | 36.28 | N  |
| ATOM   | 2654 | N   | GLY | A     | 346 | 37.280 | 59.332 | 37.870 | 1.00 | 30.83 | N  |
| ATOM   | 2655 | CA  | GLY | A     | 346 | 38.114 | 60.504 | 37.789 | 1.00 | 30.66 | C  |
| ATOM   | 2656 | C   | GLY | A     | 346 | 39.345 | 60.195 | 37.001 | 1.00 | 30.25 | C  |
| ATOM   | 2657 | O   | GLY | A     | 346 | 40.147 | 61.066 | 36.745 | 1.00 | 30.00 | O  |
| ATOM   | 2658 | N   | ARG | A     | 347 | 39.454 | 58.953 | 36.564 | 1.00 | 30.42 | N  |
| ATOM   | 2659 | CA  | ARG | A     | 347 | 40.652 | 58.496 | 35.923 | 1.00 | 30.66 | C  |
| ATOM   | 2660 | C   | ARG | A     | 347 | 40.389 | 57.879 | 34.566 | 1.00 | 30.89 | C  |
| ATOM   | 2661 | O   | ARG | A     | 347 | 41.033 | 58.241 | 33.588 | 1.00 | 30.30 | O  |
| ATOM   | 2662 | CB  | ARG | A     | 347 | 41.350 | 57.526 | 36.860 | 1.00 | 30.88 | C  |
| ATOM   | 2663 | CG  | ARG | A     | 347 | 41.786 | 58.177 | 38.171 | 1.00 | 30.97 | C  |
| ATOM   | 2664 | CD  | ARG | A     | 347 | 43.129 | 57.701 | 38.636 | 1.00 | 31.35 | C  |
| ATOM   | 2665 | NE  | ARG | A     | 347 | 43.128 | 56.255 | 38.597 | 1.00 | 30.88 | N  |
| ATOM   | 2666 | CZ  | ARG | A     | 347 | 44.088 | 55.482 | 38.128 | 1.00 | 29.55 | C  |
| ATOM   | 2667 | NH1 | ARG | A     | 347 | 45.237 | 55.962 | 37.667 | 1.00 | 28.44 | N  |
| ATOM   | 2668 | NH2 | ARG | A     | 347 | 43.876 | 54.181 | 38.147 | 1.00 | 29.95 | N  |
| ATOM   | 2669 | N   | TYR | A     | 348 | 39.446 | 56.953 | 34.480 | 1.00 | 31.67 | N  |
| ATOM   | 2670 | CA  | TYR | A     | 348 | 39.143 | 56.377 | 33.176 | 1.00 | 32.27 | C  |
| ATOM   | 2671 | C   | TYR | A     | 348 | 37.726 | 56.574 | 32.689 | 1.00 | 33.10 | C  |
| ATOM   | 2672 | O   | TYR | A     | 348 | 37.425 | 56.212 | 31.557 | 1.00 | 33.12 | O  |
| ATOM   | 2673 | CB  | TYR | A     | 348 | 39.422 | 54.896 | 33.154 | 1.00 | 31.96 | C  |
| ATOM   | 2674 | CG  | TYR | A     | 348 | 40.860 | 54.527 | 33.253 | 1.00 | 32.06 | C  |
| ATOM   | 2675 | CD1 | TYR | A     | 348 | 41.652 | 54.424 | 32.114 | 1.00 | 31.60 | C  |
| ATOM   | 2676 | CD2 | TYR | A     | 348 | 41.435 | 54.256 | 34.483 | 1.00 | 31.75 | C  |
| ATOM   | 2677 | CE1 | TYR | A     | 348 | 42.980 | 54.061 | 32.203 | 1.00 | 31.08 | C  |
| ATOM   | 2678 | CE2 | TYR | A     | 348 | 42.761 | 53.897 | 34.580 | 1.00 | 32.11 | C  |
| ATOM   | 2679 | CZ  | TYR | A     | 348 | 43.530 | 53.800 | 33.438 | 1.00 | 31.05 | C  |
| ATOM   | 2680 | OH  | TYR | A     | 348 | 44.845 | 53.427 | 33.544 | 1.00 | 29.83 | O  |
| ATOM   | 2681 | N   | ASN | A     | 349 | 36.850 | 57.137 | 33.507 | 1.00 | 34.48 | N  |
| ATOM   | 2682 | CA  | ASN | A     | 349 | 35.465 | 57.275 | 33.083 | 1.00 | 35.73 | C  |
| ATOM   | 2683 | C   | ASN | A     | 349 | 35.037 | 58.643 | 32.595 | 1.00 | 36.60 | C  |
| ATOM   | 2684 | O   | ASN | A     | 349 | 35.757 | 59.640 | 32.508 | 1.00 | 37.31 | O  |
| ATOM   | 2685 | CB  | ASN | A     | 349 | 34.542 | 56.900 | 34.212 | 1.00 | 35.62 | C  |
| ATOM   | 2686 | CG  | ASN | A     | 349 | 34.635 | 57.864 | 35.353 | 1.00 | 37.08 | C  |
| ATOM   | 2687 | OD1 | ASN | A     | 349 | 35.398 | 58.840 | 35.308 | 1.00 | 36.55 | O  |
| ATOM   | 2688 | ND2 | ASN | A     | 349 | 33.861 | 57.604 | 36.403 | 1.00 | 39.78 | N  |
| ATOM   | 2689 | OXT | ASN | A     | 349 | 33.861 | 58.757 | 32.276 | 1.00 | 38.11 | O  |
| TER    | 2690 |     | ASN | A     | 349 |        |        |        |      |       |    |
| HETATM | 2691 | FE  | FE2 | A1350 |     | 23.364 | 27.586 | 28.889 | 1.00 | 32.45 | FE |
| HETATM | 2692 | C1  | AKG | A1351 |     | 22.523 | 25.412 | 27.792 | 1.00 | 37.04 | C  |
| HETATM | 2693 | O1  | AKG | A1351 |     | 23.535 | 26.092 | 27.914 | 1.00 | 39.03 | O  |
| HETATM | 2694 | O2  | AKG | A1351 |     | 22.557 | 24.216 | 27.226 | 1.00 | 37.33 | O  |

|         |      |      |      |       |        |        |        |      |       |   |
|---------|------|------|------|-------|--------|--------|--------|------|-------|---|
| HETATM  | 2695 | C2   | AKG  | A1351 | 21.186 | 25.964 | 28.297 | 1.00 | 35.25 | C |
| HETATM  | 2696 | O5   | AKG  | A1351 | 21.175 | 27.063 | 28.807 | 1.00 | 33.44 | O |
| HETATM  | 2697 | C3   | AKG  | A1351 | 19.937 | 25.139 | 28.167 | 1.00 | 36.11 | C |
| HETATM  | 2698 | C4   | AKG  | A1351 | 18.848 | 25.738 | 29.055 | 1.00 | 36.50 | C |
| HETATM  | 2699 | C5   | AKG  | A1351 | 17.464 | 25.331 | 28.632 | 1.00 | 35.97 | C |
| HETATM  | 2700 | O3   | AKG  | A1351 | 17.276 | 24.627 | 27.656 | 1.00 | 36.64 | O |
| HETATM  | 2701 | O4   | AKG  | A1351 | 16.432 | 25.771 | 29.338 | 1.00 | 36.31 | O |
| HETATM  | 2702 | S    | SO4  | A1352 | 0.300  | 25.196 | 43.477 | 1.00 | 80.75 | S |
| HETATM  | 2703 | O1   | SO4  | A1352 | 1.094  | 26.117 | 44.306 | 1.00 | 78.50 | O |
| HETATM  | 2704 | O2   | SO4  | A1352 | 1.221  | 24.413 | 42.644 | 1.00 | 78.51 | O |
| HETATM  | 2705 | O3   | SO4  | A1352 | -0.470 | 24.282 | 44.334 | 1.00 | 79.54 | O |
| HETATM  | 2706 | O4   | SO4  | A1352 | -0.640 | 25.951 | 42.633 | 1.00 | 78.07 | O |
| HETATM  | 2707 | S    | SO4  | A1353 | 1.825  | 28.603 | 29.515 | 1.00 | 77.38 | S |
| HETATM  | 2708 | O1   | SO4  | A1353 | 3.041  | 29.212 | 30.061 | 1.00 | 76.05 | O |
| HETATM  | 2709 | O2   | SO4  | A1353 | 2.144  | 27.528 | 28.574 | 1.00 | 75.24 | O |
| HETATM  | 2710 | O3   | SO4  | A1353 | 1.090  | 28.086 | 30.675 | 1.00 | 76.52 | O |
| HETATM  | 2711 | O4   | SO4  | A1353 | 1.011  | 29.586 | 28.783 | 1.00 | 76.04 | O |
| HETATM  | 2712 | S    | SO4  | A1354 | 34.403 | 30.284 | 38.043 | 1.00 | 78.17 | S |
| HETATM  | 2713 | O1   | SO4  | A1354 | 34.921 | 31.567 | 38.516 | 1.00 | 75.93 | O |
| HETATM  | 2714 | O2   | SO4  | A1354 | 35.240 | 29.158 | 38.450 | 1.00 | 77.42 | O |
| HETATM  | 2715 | O3   | SO4  | A1354 | 33.112 | 30.084 | 38.686 | 1.00 | 75.59 | O |
| HETATM  | 2716 | O4   | SO4  | A1354 | 34.303 | 30.307 | 36.581 | 1.00 | 74.60 | O |
| HETATM  | 2717 | O    | HOH  | Z 1   | 25.824 | 26.442 | 26.175 | 1.00 | 46.43 | O |
| HETATM  | 2718 | O    | HOH  | Z 2   | 27.811 | 27.709 | 24.637 | 1.00 | 41.32 | O |
| HETATM  | 2719 | O    | HOH  | Z 3   | 27.367 | 30.233 | 25.742 | 1.00 | 38.18 | O |
| CONNECT | 1478 | 2691 |      |       |        |        |        |      |       |   |
| CONNECT | 1498 | 2691 |      |       |        |        |        |      |       |   |
| CONNECT | 2167 | 2691 |      |       |        |        |        |      |       |   |
| CONNECT | 2691 | 2696 | 2693 | 1478  | 2167   | 1498   |        |      |       |   |
| CONNECT | 2692 | 2693 | 2694 | 2695  |        |        |        |      |       |   |
| CONNECT | 2693 | 2692 | 2691 |       |        |        |        |      |       |   |
| CONNECT | 2694 | 2692 |      |       |        |        |        |      |       |   |
| CONNECT | 2695 | 2692 | 2696 | 2697  |        |        |        |      |       |   |
| CONNECT | 2696 | 2691 | 2695 |       |        |        |        |      |       |   |
| CONNECT | 2697 | 2695 | 2698 |       |        |        |        |      |       |   |
| CONNECT | 2698 | 2697 | 2699 |       |        |        |        |      |       |   |
| CONNECT | 2699 | 2698 | 2700 | 2701  |        |        |        |      |       |   |
| CONNECT | 2700 | 2699 |      |       |        |        |        |      |       |   |
| CONNECT | 2701 | 2699 |      |       |        |        |        |      |       |   |
| CONNECT | 2702 | 2703 | 2704 | 2705  | 2706   |        |        |      |       |   |
| CONNECT | 2703 | 2702 |      |       |        |        |        |      |       |   |
| CONNECT | 2704 | 2702 |      |       |        |        |        |      |       |   |
| CONNECT | 2705 | 2702 |      |       |        |        |        |      |       |   |
| CONNECT | 2706 | 2702 |      |       |        |        |        |      |       |   |
| CONNECT | 2707 | 2708 | 2709 | 2710  | 2711   |        |        |      |       |   |
| CONNECT | 2708 | 2707 |      |       |        |        |        |      |       |   |
| CONNECT | 2709 | 2707 |      |       |        |        |        |      |       |   |
| CONNECT | 2710 | 2707 |      |       |        |        |        |      |       |   |
| CONNECT | 2711 | 2707 |      |       |        |        |        |      |       |   |
| CONNECT | 2712 | 2713 | 2714 | 2715  | 2716   |        |        |      |       |   |

CLAIMS

1. A method of identifying, screening, characterising or designing a chemical entity which mimics or binds to FIH, which method comprises comparing a structural model of FIH with a structural model for said chemical entity, wherein said structural model of FIH is derived from structural factors or structural coordinates determined by subjecting to X-ray diffraction measurements a crystal comprising FIH.
2. Use of the structural co-ordinates obtainable by subjecting a crystal comprising FIH to X-ray diffraction measurements and deducing the structural co-ordinates from the diffraction measurements, to identify, screen, characterise, design or modify a chemical entity.
3. A method or use according to claim 1 or 2 in which the structural coordinates are those shown in Table 3.
4. A method or use according to any one of the preceding claims, wherein said chemical entity binds to FIH.
5. A method or use according to any one of the preceding claims, wherein said chemical entity is selected to inhibit the asparaginyl hydroxylase activity of FIH.
6. A method or use according to any one of the preceding claims further comprising contacting said chemical entity with HIF or a fragment thereof or a homologue of either thereof incorporating asparagine 803 with FIH or a homologue thereof which maintains the asparaginyl hydroxylase activity of FIH and monitoring for hydroxylation of asparagine 803.
7. A chemical entity identified by a method for use according to any one of the preceding claims, wherein said chemical entity inhibits the asparaginyl hydroxylase activity of FIH.
8. A chemical entity according to claim 7 wherein said chemical entity inhibits hydroxylation of the asparagine position 803 of HIF by FIH.
9. A chemical entity according to claim 7 wherein said chemical entity inhibits dimerisation of FIH.



10. A chemical entity according to claim 9 wherein said chemical entity binds to residues that form the dimerisation interface of FIH, selected from residues 330 to 346 of FIH.

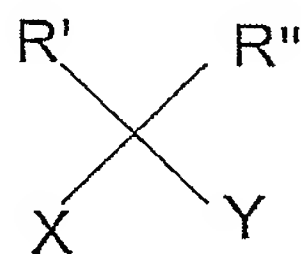
11. A chemical entity according to claim 7 wherein said chemical entity  
5 binds to iron, or prevents Fe(II) binding to FIH.

12. A chemical entity according to claim 11, wherein said chemical entity is a compound selected from a thiol, alcohol, phenol, carboxylate, hydroxamate, imidazole or other heterocyclic compound, that binds to iron.

13. A chemical entity according to claim 7 wherein said chemical entity  
10 disrupts 2-oxoglutarate binding to FIH.

14. A chemical entity according to claim 13, wherein said chemical entity is R-entimer of N-oxaloylalanine, procollagen prolyl-hydroxylase and a PHD isozyme.

15. A chemical entity according to claim 13, wherein said chemical entity  
15 is a compound of the formula



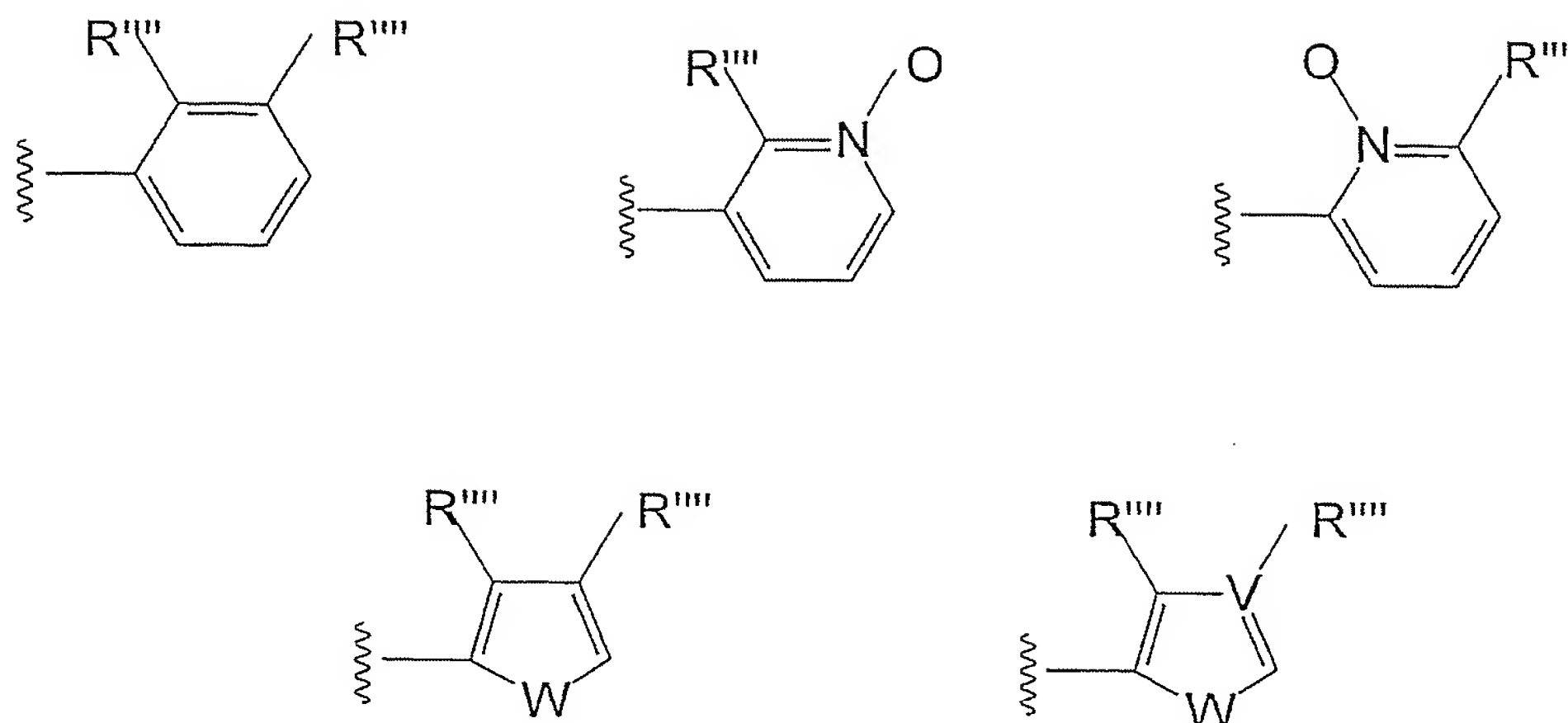
(I)

20 wherein each of R' and R'', which may be the same or different, is H, F or C<sub>1</sub> to C<sub>3</sub> alkyl or substituted alkyl, CH<sub>2</sub>OH, CH<sub>2</sub>CO<sub>2</sub>H or CONH<sub>2</sub>, X is COOH, SOOH, or CONHH or an ester thereof, or other group which forms a favourable interaction with one or more of the side chains of Lys-214, Thr-196 and Tyr-145,

Y is - (CR'''R''')<sub>n</sub>Z, where Z is

25 - NR'''COCOOH, - NR'''CSCOOH, - NR'''COCOSH,  
- CHSR'''CONR'''R''', - CHOR'''CONR'''OR''', - CHSR'''CONR'''OR''' or  
- CHOR'''CONR'''NR'''OR''', wherein each R''', which may be the same or different, is H, alkyl, OH or O-alkyl, n is 0 to 3, or

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5 wherein R'''' is OH, OR''' or NHCOR''', and W is S, NH, or O;

16. A chemical entity according to claim 13 or 15 wherein said chemical entity interferes with the interactions at residues 214, 196 and 145 of FIH, or which interrupts the interactions of 2OG with residues 281, 186, 188, 207 or 196 of FIH.

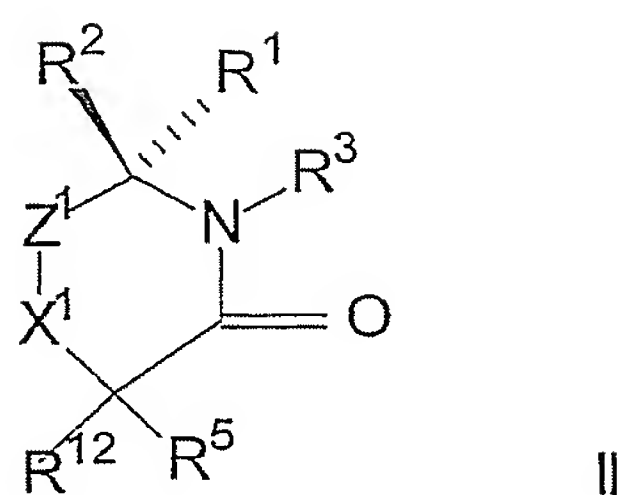
17. A chemical entity according to claim 16 wherein said chemical entity  
10 interrupts binding of FIH for Asn 803 of HIF, preferably, by interfering with binding of HIF at residues 102, 239 or 238 of HIF.

18. A chemical entity according to claim 17 which interferes with Site 1 binding of CAD of HIF to FIH and which exploits electrostatic, hydrogen binding and/or hydrophobic interactions with one or more residues selected from 102, 104,  
15 106, 201, 202, 147, 239, 299-303, 313, 317, 318, 321, 324, 238, 296 or 321 to 324 of FIH.

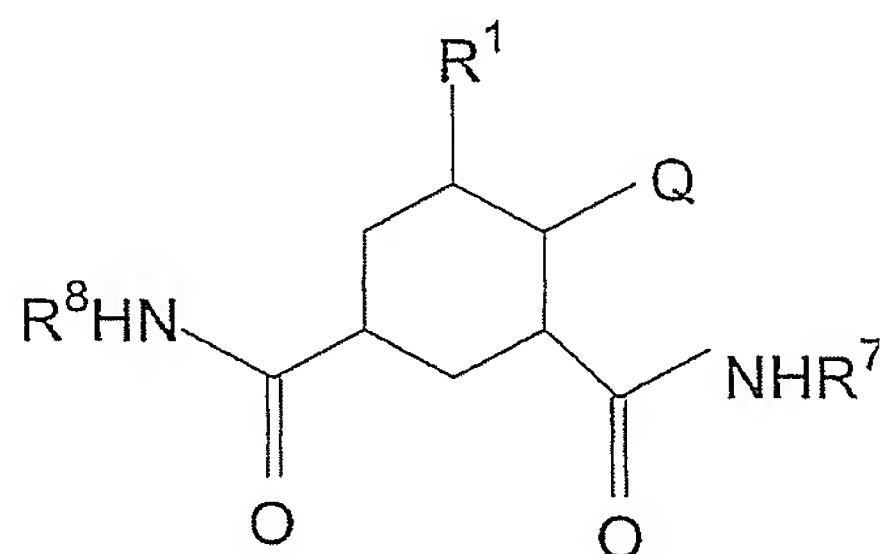
19. A chemical entity according to claim 17 wherein said chemical entity interferes with binding of CAD of HIF to FIH at Site 2, and exploits electrostatic, hydrogen binding and/or hydrophobic interactions with residues 149, 150, 151, 152,  
20 159, 162, 163, 167, 181, 182, 183, 184 or 185.

20. A chemical entity according to claim 17 wherein said chemical entity is a compound of the formula

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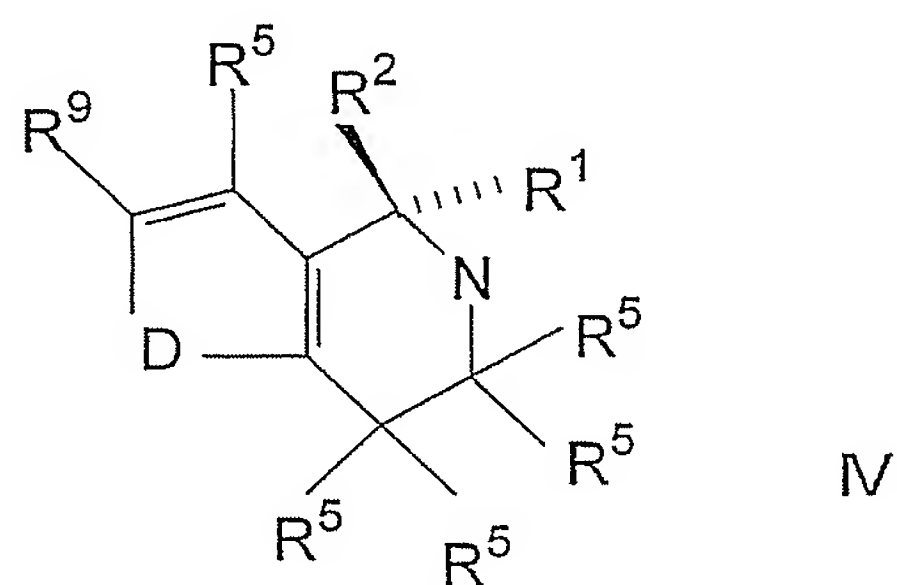


21. A chemical entity according to claim 17, wherein said chemical entity is a compound of the formula



5

22. A chemical entity according to claim 17 wherein said chemical entity is a compound of the formula



23. A chemical entity according to claim 17 wherein said chemical entity is a compound of the formula



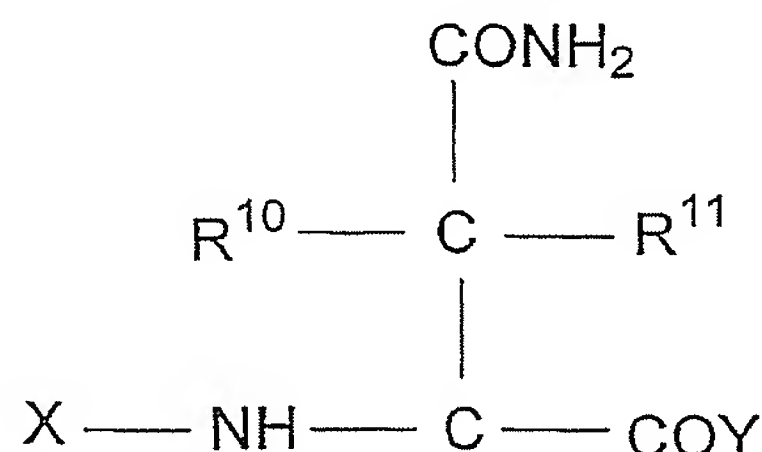
where X is as defined above, B is a linker group and C is an entity binding to part of the CAD binding site of FIH;

24. A chemical entity according to claim 17 wherein said chemical entity is a compound of the formula



where X and B are as defined above and E is an entity binding to part of the CAD when bonded to HIF.

25. A chemical entity according to claim 7 wherein said chemical entity is a compound of the formula



wherein X represents a valine residue or an analogue thereof and Y represents an alanine residue or an analogue thereof,  $\text{R}^{10}$  is fluorine or  $\text{C}_1 - \text{C}_3$  alkyl, and  $\text{R}^{11}$  is fluorine,  $\text{C}_1 - \text{C}_3$  alkyl or hydrogen or a corresponding compound  $\text{R}^{11}$  is absent or  $\text{R}^{10}$  and  $\text{R}^{11}$  form a methylene group.

26. A chemical entity according any of one of claims 7 to 25 for use in a method of treatment.

27. A chemical entity according to any of claims 7 to 25 for use in the treatment of a condition associated with increased or decreased HIF levels or activity or the treatment of a condition where it is desired to modulate HIF activity.



28. A chemical entity according to claim 27 wherein said condition is ischaemia, wound healing, auto-, allo- or xeno-transplantation, systemic high blood pressure, cancer or an inflammatory disorder.

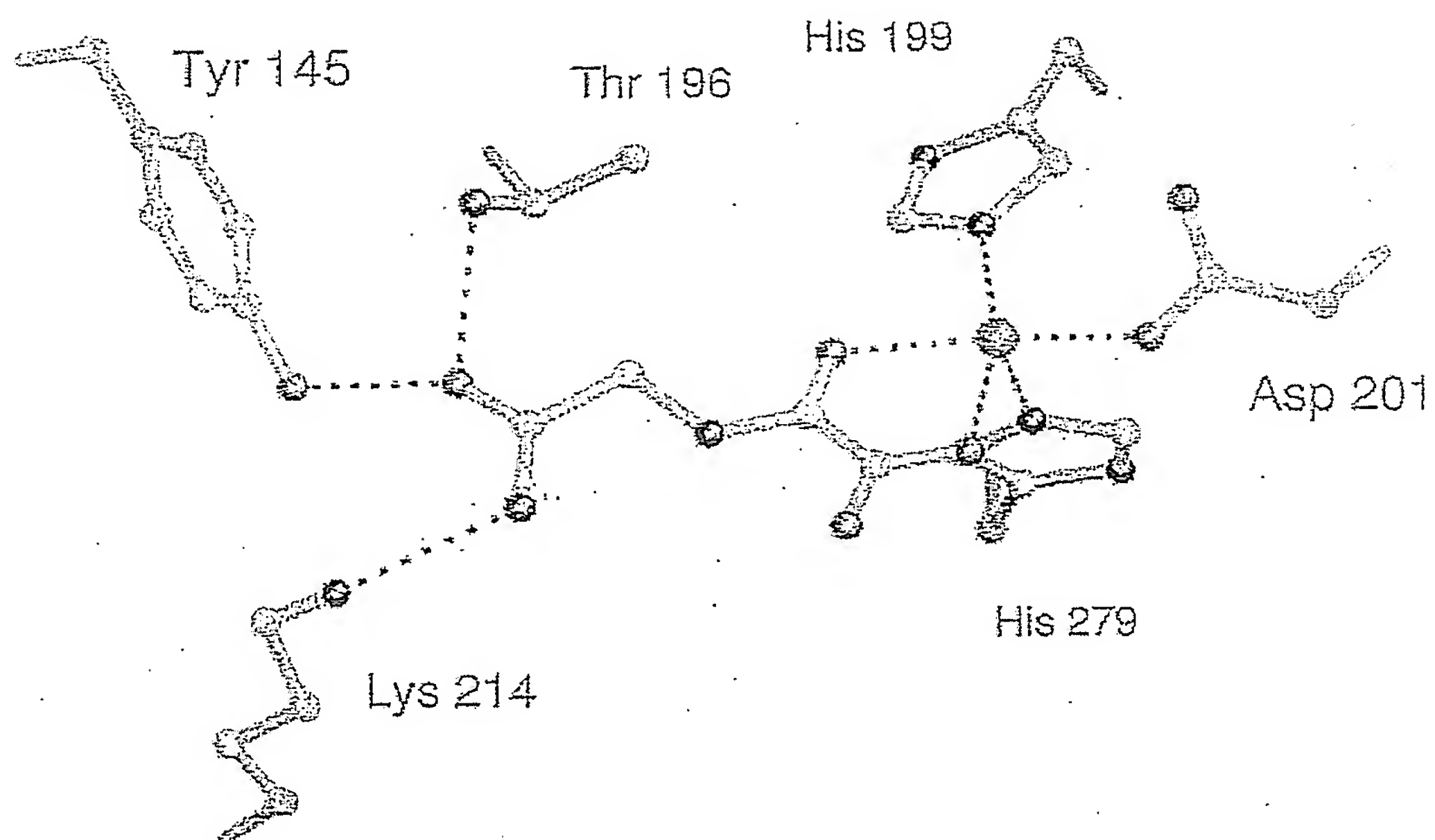


FIGURE 1

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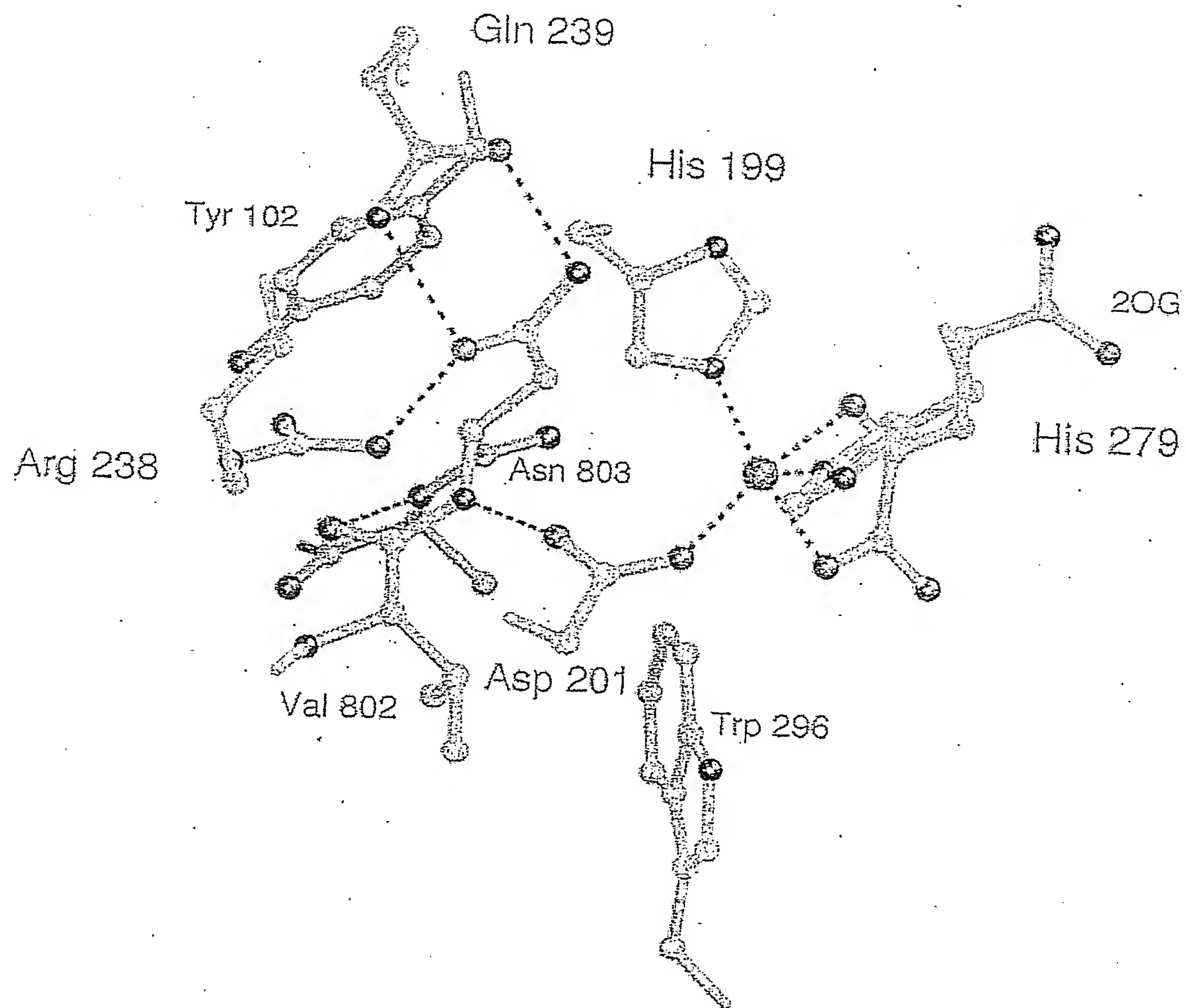


FIGURE 2

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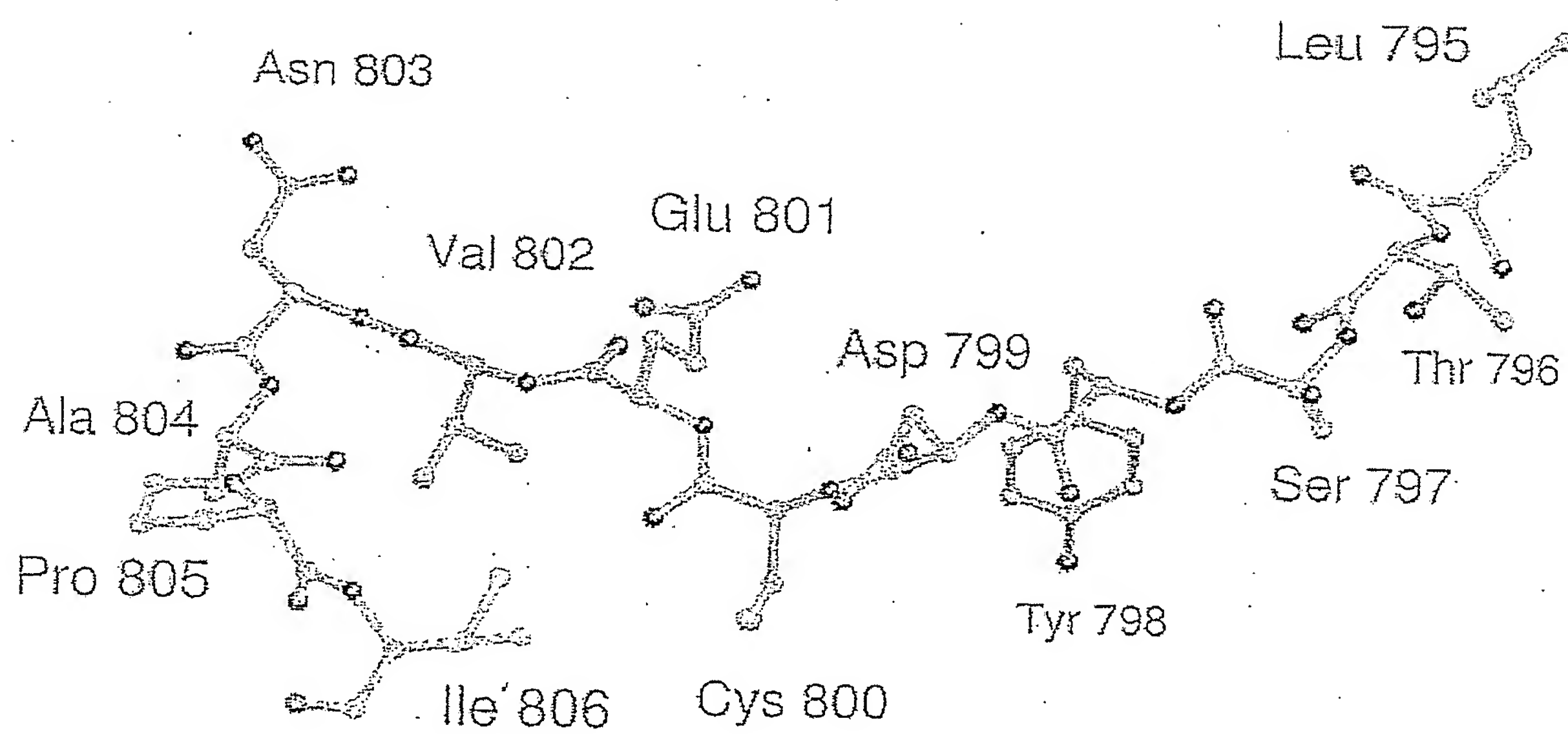


FIGURE 3



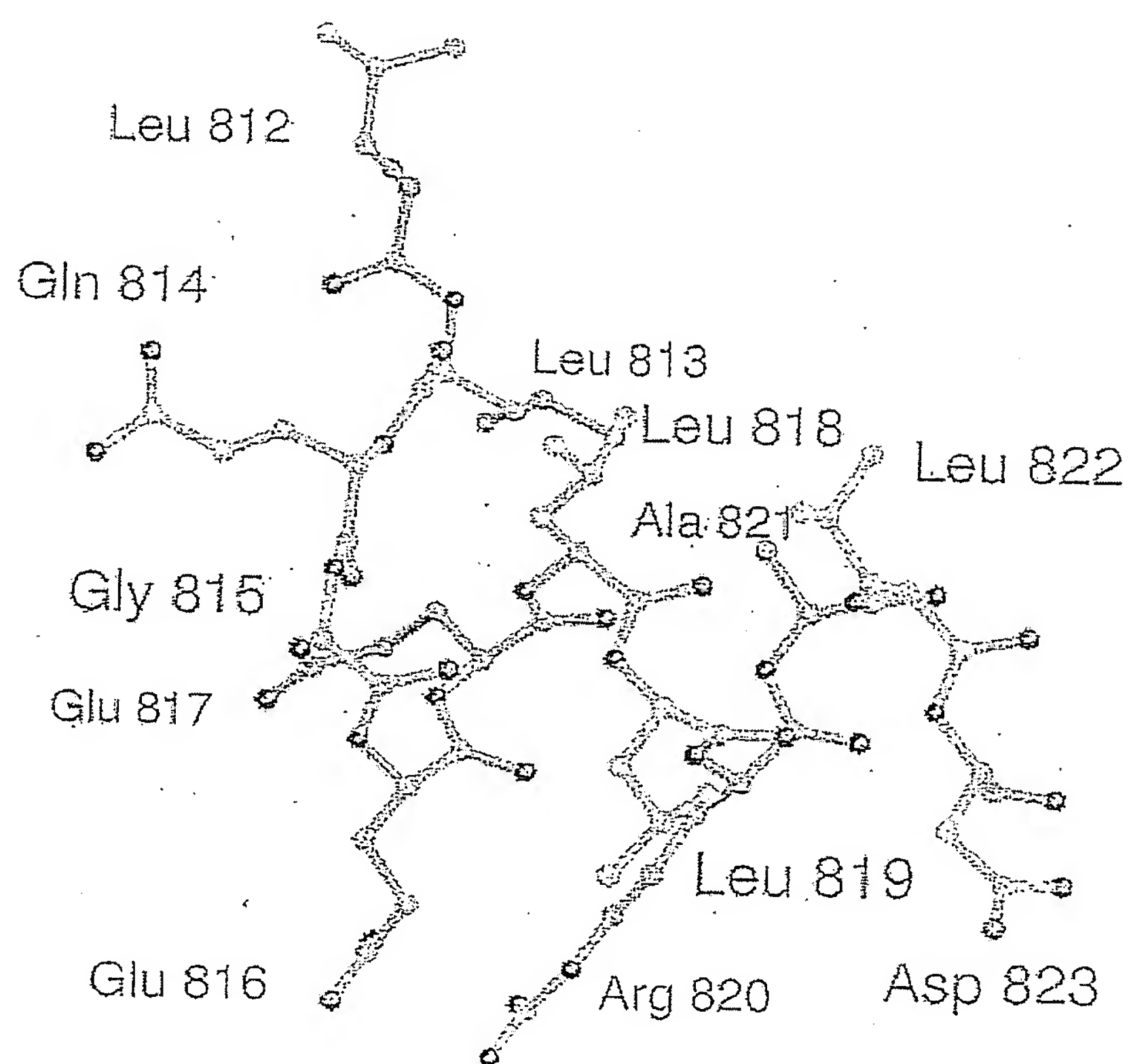


FIGURE 4

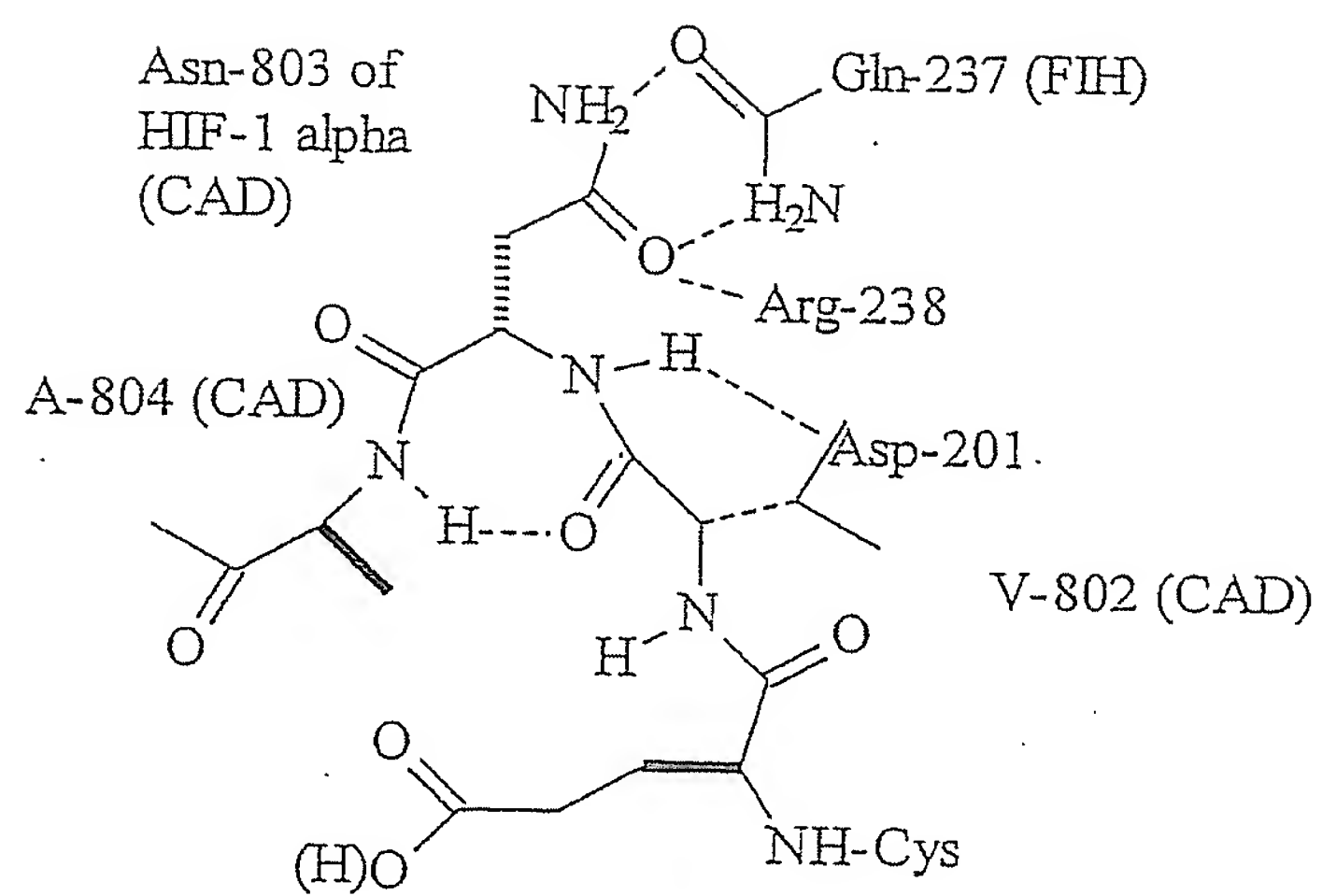


FIGURE 5

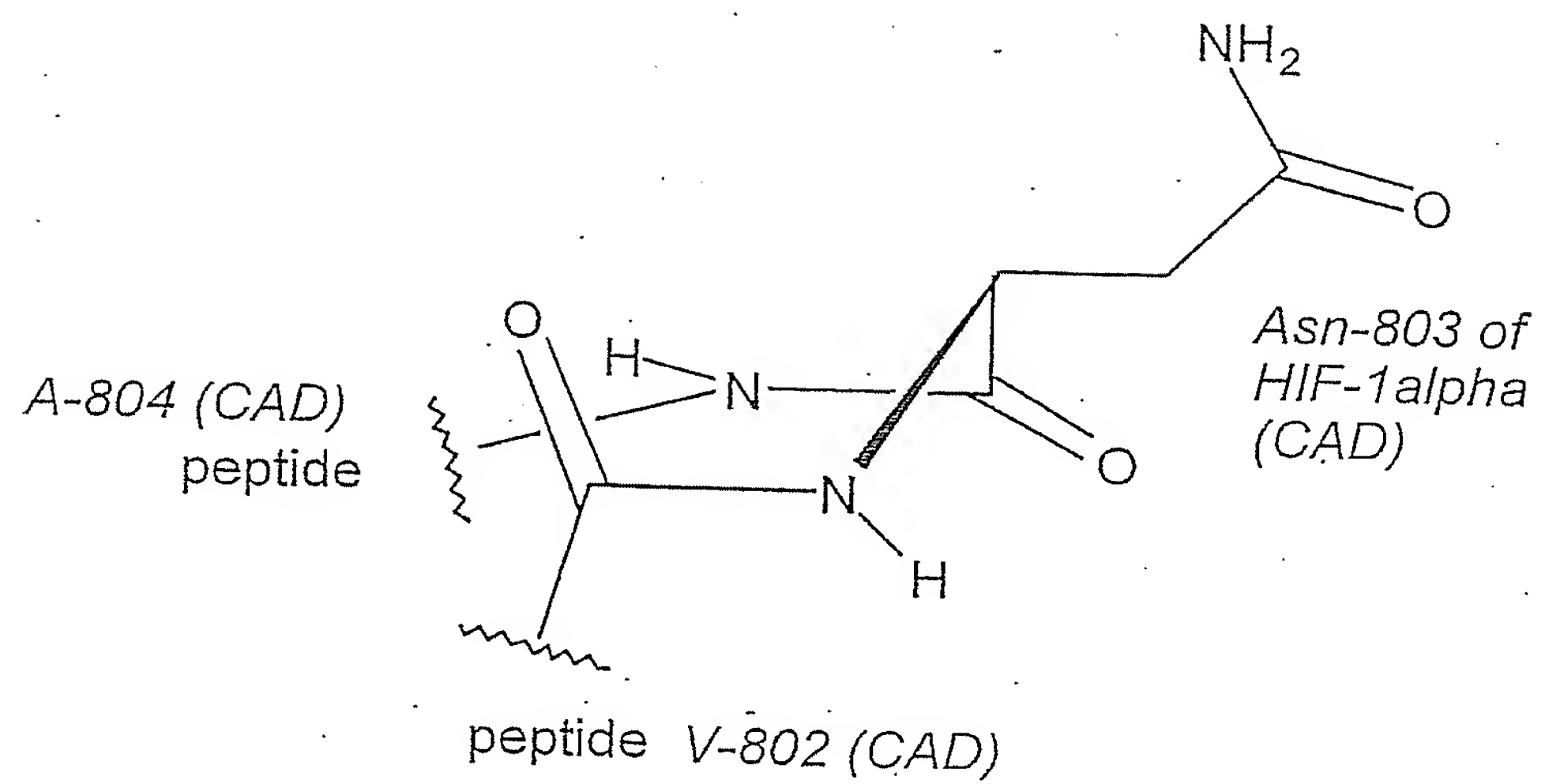


FIGURE 6